SUPPORTING INFORMATION

FOR

Site Specific Carboxylation of Abnormal Anionic N-Heterocyclic Carbenes

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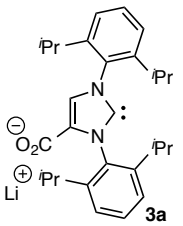
Contents

1. GENERAL

Solvents and reagents were ACS reagent grade and used without further purification unless noted below. Tetrahydrofuran (THF) and diethyl ether (Et_2O) were passed through a column of molecular sieves and stored under argon. All reactions were carried out in flame-dried glassware. *N,N'*-bis-(2,6-diisopropylphenyl)-imidazol-2-ylidene **1a**[1] and *N,N'*-diisopropyl-imidazol-2-ylidene **1b**[2] were prepared according to literature procedures. Dry CO_2 was obtained by passing sublimed dry ice through concentrated sulfuric acid followed by a drying tube charged with $CaCl_2$.

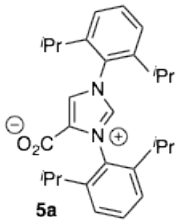
^{1}H Nuclear magnetic resonance (NMR) spectra were obtained either at 300 or 500 MHz, and ^{13}C NMR spectra at 75 or 125 MHz. Chemical shifts are reported in parts per million (ppm, δ), and referenced to residual solvent. Coupling constants are reported in Hertz (Hz). Spectral splitting patterns are designated as s, singlet; d, doublet; t, triplet; q, quartet; p, pentet; m, multiplet; comp, complex; app, apparent; hom, higher order multiplet; and br, broad. Infrared (IR) spectra were obtained using a Thermo Electron Nicolet 380 FT-IR using a silicon (Si) crystal in an attenuated total reflectance (ATR) tower and reported as wavenumbers (cm^{-1}). High and Low resolution electrospray ionization (ESI) measurements were made with a Bruker MicroTOF II mass spectrometer. Analytical thin layer chromatography (TLC) was performed using EMD 250 micron 60 F_{254} silica gel plates, visualized with UV light and stained with a *p*-anisaldehyde solution.

2. EXPERIMENTAL PROCEDURES



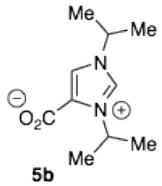
3a

Lithium *N,N*-Bis-(2,6-diisopropylphenyl)-imidazol-2-yliden-4-carboxylate (3a). A solution of **1a** (66.7 mg, 0.17 mmol) in dry, degassed THF (2 mL) was stirred for 20 minutes at room temperature. A solution of ^{n}BuLi (0.172 mmol, 0.13 mL, 1.32 M in hexanes) was added dropwise over 10 minutes, and stirred for 2 h until the solution turned bright orange. The resulting solution was then cooled to -78 °C, at which point dried CO_2 (passing through two columns of anhydrous $CaSO_4$) was condensed into the reaction mixture for 30 minutes. The Schlenk line needle was then removed from the solvent to provide an atmosphere of CO_2 as the reaction was removed from the cooling bath. An outlet needle was affixed and the mixture was allowed to warm to room temperature over 2 h. The completed reaction mixture was immediately concentrated under reduced pressure and dried under high vacuum (~0.1 atm) at 70 °C for 3 h to afford 68 mg (90%) of **3a** as a light red solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (s, 1H), 7.59 (t, *J* = 8 Hz, 1H), 7.47 (t, *J* = 8 Hz, 1H), 7.36 (d, *J* = 8 Hz, 2H), 7.29 (d, *J* = 8 Hz, 2H), 2.49 (m, 4H), 1.32 (d, *J* = 7 Hz, 6H), 1.29 (d, *J* = 7 Hz, 6H), 1.19 (d, *J* = 7 Hz, 6H), 1.14 (d, *J* = 7 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ23.7, 24.1, 24.7, 24.9, 29.1, 29.3, 29.4, 77.4, 124.3, 125.0, 125.8, 130.0, 131.1, 132.4, 139.0, 144.8, 145.4, 157.1; IR ($CDCl_3$) 2966, 1655, 1529, 1464, 1331, 1216; HRMS (ESI) *m/z* anion: 431.2726 [$C_{28}H_{35}N_2O_2$ requires 431.2704].



5a

***N,N*-Bis-(2,6-diisopropylphenyl)-imidazolium-5-carboxylate (5a).** A solution of **1a** (356 mg, 0.92 mmol) in dry, degassed THF (5.7 mL) under argon atmosphere was stirred for 10 min at room temperature. A solution of ^{n}BuLi (0.93 mmol, 0.58 mL, 1.6 M in hexanes) was then added dropwise, and the solution was stirred for an additional 2 h at room temperature until it became a bright orange color. The resulting solution was cooled to -78 ˚C at which point CO_2 was condensed into the reaction. After 10 to 15 min the reaction flask was equipped with a CO_2 filled balloon and disconnected from the Schlenk line. The reaction was allowed to warm to room temperature over 2 h by removal of the cooling bath. The resulting light yellow suspension was filtered and washed with Et_2O (2 x 6 mL) to provide 405 mg (>95%) of **5a** as a light yellow solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.83 (d, *J* = 2 Hz, 1H), 7.81 (d, *J* = 2 Hz, 1H), 7.59 (t, *J* = 8 Hz, 1H), 7.48 (t, *J* = 8 Hz, 1H), 7.36 (d, *J* = 8 Hz, 2H), 7.29 (d, *J* = 8 Hz, 2H), 2.50 (m, 4H), 1.33 (d, *J* = 7Hz, 6H), 1.29 (d, *J* = 7 Hz, 6H), 1.17 (d, *J* = 7Hz, 6H), 1.14 (d, *J* = 7 Hz, 6H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 23.7, 24.0, 24.7, 24.9, 29.0, 29.4, 124.3, 124.9, 125.4, 125.9, 131.0, 132.3, 134.4, 135.5, 144.7, 145.3, 148.1, 166.9; IR (neat) 3155, 2961, 2742, 1653, 1525, 1439, 1331, 1297, 1259, 1230, 864, 795, 755, 504; HRMS (ESI) *m/z* 433.2945 [$C_{28}H_{37}N_2O_2$ (M+1) requires 433.2850].



5b

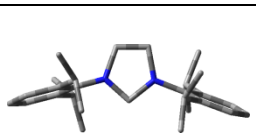
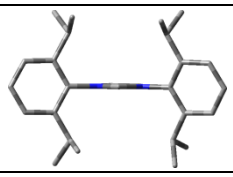
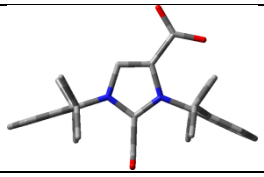
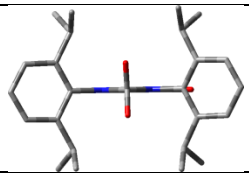
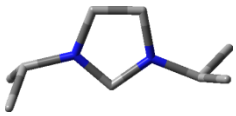
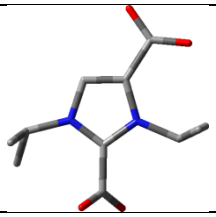
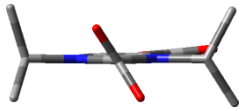
***N,N*-Diisopropyl-imidazolium-5-carboxylate (5b).** ^{n}BuLi (0.78 mmol, 1.32 mmol, 1.7 M in hexanes) was added dropwise to a solution of **1b** (200 mg, 1.31 mmol) in dry, degassed Et_2O (5 mL) at 0 ˚C under argon atmosphere and stirred for 2 h. The mixture was cooled to -78 ˚C and CO_2 was condensed into the reaction. After 10 min the reaction flask was equipped with a CO_2 filled balloon and disconnected from the Schlenk line. The reaction was allowed to warm to room temperature by removal of the cooling bath and stirred for 14 hr. The resulting pale yellow suspension was filtered and washed with Et_2O (2 x 5 mL) to provide 199 mg (77%) of **5b** as a yellow solid . ^{1}H NMR (300 MHz, $CDCl_3$) δ 9.90 (br s, 1H), 7.62 (br s, 1H), 6.08 (m, 1H), 4.91 (m, 1H), 1.61 (s, 3H), 1.59 (s, 3H), 1.58 (s, 3H), 1.56 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 23.3, 23.5, 50.7, 52.7, 84.7, 120.8, 188.7; IR (neat) 3399, 2969, 1631, 1374, 1182; HRMS (ESI) *m/z* 197.1319 [$C_{10}H_{17}N_2O_2$ (M+1) requires 197.1285].

3. Calculation Setup

We chose B3LYP/6-311++g(d,p)[3] as the DFT method to study the gas phase reactivity between CO_2 and NHDCs (with *N*,*N*-diisopropyl (**2b**, **3b**, **3´b**, **4b**, **5b**, all are anions without Li ion, **3´** meaning that the CO_2 binds at C2) and *N*,*N*-diisopropylphenyl substitutions (**2a**, **3a**, **3´a**, **4a**, **5a** all are anions without Li ion)) using GAUSSIAN 09 package.[4] All the energy minimum structures are given below. The binding energy are computed using electronic energy following the equation: Eb = E(NHDC_CO_2) - E(NHDC) - E(CO_2).

4. Optimized Structures of NHDC Molecules Binding with CO_2

Figure S1. Optimized NHDC molecules before and after reacting with CO_2. Hydrogen atoms are hidden for clarity. Red is O, blue is N, and grey is C.

Before reaction		After binding with two CO_2 molecules	
Top	Side	Top	Side
NHDC **2a**		**4a**	
			
NHDC **2b**		**4b**	
			

5. Calculated Geometric Parameters of NHDC Molecules Binding with CO_2

Table S1. Geometric parameters[1] of NHDC molecules binding with CO_2

	One CO_2 (3 at C5, 3' at C2)[4]				Two CO_2 (4)			
	at C2		at C5		at C2		at C5	
	∠OCO[2]	dC-C[3]	∠OCO	dC-C	∠OCO	dC-C	∠OCO	dC-C
1b	129.8	1.544	129.2	1.540	131.7	1.553	130.6	1.553
2a	131.4	1.544	130.4	1.535	132.2	1.550	131.7	1.543

1. Electronic energy, in kJ/mol.
2. Angle in degree.
3. Bond distance in Å.
4. Binding at C2 is named 3'a or 3'b.

6. TOTAL ENERGY OF NHDC MOLECULES BINDING WITH CO_2

Table S2. Calculated electronic energy (Hartree) of NHDC molecules binding with CO_2. CO_2 energy is -188.6469148 Hartree.

anion	no CO_2	one CO_2 at C2	one CO_2 at C5	two CO_2
1b	-461.5609104	-650.2599307	-650.2759	-838.9552793
2a	-1159.724256	-1348.414613	-1348.429675	-1537.105602

7. OPTIMIZED GEOMETRIC COORDINATES OF CALCULATED MOLECULES

2b

-1 1 (charge and spin multiplicity)

N	0.97102400	-0.58038300	-0.46168600
C	0.02239200	-0.21719300	-1.46445100
C	-0.44735900	0.95642900	-0.93428000
N	0.20151600	1.23549900	0.29879500
C	1.10424300	0.26814400	0.60883400
H	-1.19625300	1.64163100	-1.31158900
C	-0.05107500	2.41048700	1.12461100
H	-0.83627800	2.97354100	0.60549700
C	1.19278700	3.30531000	1.22538700
H	1.53451900	3.59328500	0.22750300
H	0.97777700	4.21550900	1.79943700
H	2.00114000	2.75576900	1.71277600
C	-0.57865600	2.02213000	2.51302200
H	-0.81650100	2.91431100	3.10597800
H	-1.48154700	1.41272600	2.41919900
H	0.17362500	1.43064100	3.03926700
C	1.77578300	-1.79751400	-0.55522400
H	2.39418000	-1.80200600	0.34758100
C	2.68902800	-1.75824500	-1.78768700
H	3.35529100	-0.89188100	-1.73732500
H	3.30080800	-2.66688500	-1.85219200
H	2.07998400	-1.66583700	-2.69025800
C	0.88469100	-3.04655200	-0.55985000
H	1.48939700	-3.95986500	-0.62428200
H	0.28610200	-3.08816300	0.35499400
H	0.20054400	-3.00306300	-1.41082200

3b

-1 1

N	0.82866800	-0.72693400	-0.31295200
C	-0.39875700	-0.51311000	-0.98381700
C	-0.87168400	0.65077200	-0.46276800
N	0.04570600	1.09879000	0.47574100
C	1.11628100	0.25792500	0.59013800

H	-1.78619100	1.16382800	-0.70794700
C	-0.11051000	2.32452400	1.26565100
H	-1.05162600	2.77216600	0.92961200
C	1.02851300	3.30992800	0.98152300
H	1.07243400	3.55027000	-0.08385100
H	0.88344200	4.23895500	1.54355500
H	1.98288300	2.86348200	1.26822300
C	-0.22911300	2.00309100	2.75998400
H	-0.39314700	2.91795100	3.33975000
H	-1.06395800	1.32136400	2.94171700
H	0.68601300	1.51911200	3.10759000
C	1.78984600	-1.84041000	-0.46932000
H	2.56959700	-1.57156400	0.24709300
C	2.40877000	-1.87506300	-1.87070900
H	2.85519900	-0.90514500	-2.11113500
H	3.20046300	-2.63259700	-1.90248400
H	1.64634600	-2.12180300	-2.61083000
C	1.18789500	-3.18531700	-0.04854400
H	1.96852700	-3.95489700	-0.05963600
H	0.78898500	-3.11933400	0.96851000
H	0.39192100	-3.47206700	-0.73702700
C	-1.12605900	-1.33486400	-2.06475000
O	-2.20903200	-0.82716500	-2.42931100
O	-0.57490600	-2.39237700	-2.45371200

3'b

-1 1

N	1.06941600	-0.56299900	-0.56185800
C	0.05170500	-0.20829500	-1.47404200
C	-0.41975700	0.94519600	-0.89606500
N	0.28507200	1.26549500	0.27741600
C	1.21370600	0.30633000	0.47191500
H	-1.22945300	1.59154200	-1.20269800
C	-0.02288100	2.46763600	1.07826000
H	-0.98237000	2.79867700	0.66705600
C	1.00584600	3.58128100	0.84618100
H	1.08468800	3.80855000	-0.22083700
H	0.69114900	4.49130600	1.36938100
H	1.97886600	3.25909500	1.21909700
C	-0.24084900	2.15512700	2.56196200
H	-0.63462800	3.04534000	3.06428100
H	-0.96506600	1.34494700	2.68249500
H	0.69578500	1.87098000	3.04111000
C	1.91660300	-1.75725200	-0.76251600
H	2.60530100	-1.78620500	0.08005000
C	2.69325200	-1.63010500	-2.07648400
H	3.33313100	-0.74312300	-2.06242800
H	3.32896200	-2.51005600	-2.22344200
H	2.00034500	-1.53973200	-2.91611300

C	1.05133100	-3.01958800	-0.72346800
H	1.67519100	-3.90727800	-0.87466900
H	0.55810900	-3.10742600	0.24761200
H	0.28794500	-2.97619800	-1.50371900
C	2.22438100	0.20762300	1.63506700
O	2.75628600	1.28813800	1.97395400
O	2.38490800	-0.94132500	2.09510300

4b

-1 1

N	0.89839900	-0.73411700	-0.38240600
C	-0.35010300	-0.49710400	-0.98922500
C	-0.82328400	0.63290100	-0.39919600
N	0.10339000	1.08173600	0.52433000
C	1.15303300	0.23221100	0.52547500
H	-1.75985800	1.12959400	-0.57934900
C	-0.09543800	2.32653400	1.30811900
H	-1.16288200	2.52950500	1.18269100
C	0.69833200	3.48930100	0.70275400
H	0.42809400	3.63350700	-0.34678300
H	0.46746900	4.41111800	1.24588200
H	1.76709000	3.28215000	0.77182400
C	0.17010500	2.12869600	2.80246300
H	-0.16933200	3.01871200	3.34061900
H	-0.37866800	1.26559700	3.18646200
H	1.23171400	1.99051200	3.00591200
C	1.87130400	-1.84031300	-0.63552200
H	2.65549100	-1.66053300	0.09725100
C	2.46438900	-1.73724600	-2.04277000
H	2.91628300	-0.75317200	-2.19744100
H	3.25270800	-2.48944600	-2.14899100
H	1.69463500	-1.91473600	-2.79404000
C	1.25035300	-3.20298100	-0.32275000
H	2.02713900	-3.96939200	-0.40957300
H	0.87589400	-3.22050800	0.70388500
H	0.44615700	-3.42914800	-1.02262900
C	-1.11435900	-1.25949900	-2.10536000
O	-2.24714000	-0.78020400	-2.30642400
O	-0.52647200	-2.21331500	-2.65426300
C	2.41441200	0.35220200	1.42388000
O	3.02940200	1.42716800	1.28911300
O	2.61805600	-0.63036100	2.15571800

2a

-1 1

C	0.33532400	1.32987800	-0.02465600
C	1.56042300	1.78838200	0.38096200
C	1.67298400	1.96538800	-1.92133900
N	0.47634100	1.46814600	-1.44648200

H	1.97496600	1.89322500	1.37341800
N	2.34683000	2.16115700	-0.75262400
C	3.67887600	2.66308000	-0.67808500
C	4.76401700	1.76531400	-0.76322700
C	3.89188500	4.04285600	-0.48469400
C	6.06192000	2.27818500	-0.67935600
C	5.20752800	4.51102100	-0.40344200
C	6.28693100	3.63990900	-0.50173700
H	6.90989300	1.60579800	-0.75489500
H	5.39069300	5.57198300	-0.26749200
H	7.30191400	4.02046900	-0.43959600
C	-0.58010000	1.10127900	-2.33670600
C	-1.41584500	2.09538300	-2.88191600
C	-0.79181700	-0.26030200	-2.63625300
C	-2.45475900	1.70690600	-3.73466600
C	-1.84730800	-0.60431000	-3.48586300
C	-2.67466300	0.36834100	-4.03771400
H	-3.10675400	2.46292900	-4.16122700
H	-2.02502200	-1.64878500	-3.72098900
H	-3.48838100	0.08340000	-4.69797900
C	-1.23240800	3.56844300	-2.53943700
H	-0.36735500	3.63694000	-1.88082000
C	0.08490300	-1.34908600	-2.03053600
H	0.94236200	-0.85105400	-1.57779000
C	2.72328100	5.01861600	-0.41655000
H	1.81371700	4.42417300	-0.32216900
C	4.52759100	0.27743100	-0.99182600
H	3.48968200	0.07708200	-0.72036200
C	-0.92623900	4.41428000	-3.78754600
H	-0.03250300	4.04009200	-4.29219500
H	-1.75594900	4.39823200	-4.50293100
H	-0.74856300	5.45865200	-3.50795200
C	-2.44565200	4.11928100	-1.76700000
H	-3.35989100	4.08503200	-2.37016800
H	-2.61584100	3.53857200	-0.85729000
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C	2.61335800	5.82815500	-1.72252100
H	3.50396200	6.44634300	-1.88304500
H	2.50161600	5.15799600	-2.57751400
H	1.74278900	6.49239000	-1.69117500
C	2.79414200	5.94458500	0.80995500
H	2.85559400	5.36642700	1.73585000
H	3.65984100	6.61447100	0.77204500
H	1.89673600	6.56969300	0.86176200
C	5.41458100	-0.61747400	-0.11002200
H	6.47534300	-0.53489900	-0.36963900
H	5.30560800	-0.36496300	0.94848100
H	5.12945100	-1.66665500	-0.23804500
C	4.68879300	-0.07394600	-2.48359800

H	3.99204100	0.51330900	-3.08532400
H	5.70961300	0.13014400	-2.82708200
H	4.47988500	-1.13617100	-2.65235500
C	0.62142500	-2.33350800	-3.08479500
H	-0.17971900	-2.91585800	-3.55275900
H	1.16144400	-1.80660500	-3.87625800
H	1.31141300	-3.04487600	-2.61788100
C	-0.65847800	-2.08360900	-0.89916700
H	-0.94694500	-1.36960100	-0.12488300
H	-1.55733700	-2.58596600	-1.27610900
H	-0.01133800	-2.84316400	-0.44521200

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N	0.86109200	-0.71748500	-0.38818700
C	-0.41640500	-0.54604500	-0.93270300
C	-0.87598100	0.63491900	-0.41694500
N	0.09202300	1.16582300	0.40956900
C	1.13225900	0.32130300	0.41045600
H	-1.82297200	1.11129700	-0.60179700
C	-0.04699000	2.40705700	1.21041400
H	-0.86203000	2.94768100	0.72444500
C	1.21955900	3.25975100	1.13265300
H	1.49946100	3.46081900	0.09666700
H	1.04303600	4.21531500	1.63066000
H	2.06305700	2.78080600	1.63754400
C	-0.45759800	2.07379100	2.64762700
H	-0.65231700	2.99580300	3.20037700
H	-1.36387400	1.46544400	2.66688900
H	0.33572300	1.52869300	3.16650500
C	1.86458700	-1.81474000	-0.58776000
H	2.70285000	-1.49861100	0.04227100
C	2.33985100	-1.86715600	-2.03959400
H	2.72137800	-0.89461900	-2.36298700
H	3.15305800	-2.59362600	-2.11766500
H	1.52001900	-2.17587800	-2.68788600
C	1.33424500	-3.14755400	-0.06006500
H	2.13605400	-3.88915100	-0.10834400
H	1.01674500	-3.05835800	0.98263200
H	0.49764300	-3.48304800	-0.67265200
C	-1.22889500	-1.44299800	-1.92291300
O	-2.33595700	-0.94535200	-2.16817400
O	-0.66560600	-2.48408100	-2.30265100
H	2.04712400	0.45354600	0.96129300

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C	0.35691000	1.52920300	0.01242100

C	1.57911900	1.95413400	0.42209000
C	1.65494500	1.91754000	-1.88021900
N	0.43495700	1.51667300	-1.39667400
H	1.94070400	2.10361900	1.42456800
N	2.34461700	2.18257500	-0.72263500
C	3.70263200	2.64272800	-0.69925500
C	4.74626600	1.69707900	-0.69751800
C	3.95981200	4.02611500	-0.67379500
C	6.06241800	2.16845500	-0.68005400
C	5.29317800	4.44888700	-0.65433200
C	6.33704300	3.53148300	-0.65790400
H	6.88396700	1.46077300	-0.68660400
H	5.51618000	5.51038600	-0.64116100
H	7.36552800	3.87810000	-0.64477900
C	-0.61638600	1.14002500	-2.31255500
C	-1.49143400	2.12817300	-2.79223100
C	-0.70154200	-0.19322100	-2.74627300
C	-2.43978200	1.76090300	-3.75070800
C	-1.66559600	-0.51429000	-3.70543200
C	-2.52481600	0.45309800	-4.21312700
H	-3.12897400	2.50701000	-4.13192000
H	-1.75247500	-1.53870000	-4.05166600
H	-3.26840000	0.18518200	-4.95735400
C	-1.47452400	3.55117100	-2.25071500
H	-0.61100700	3.64043100	-1.59072900
C	0.16908200	-1.29083800	-2.15002700
H	0.92160100	-0.80890000	-1.52485100
C	2.83564500	5.05494200	-0.70265100
H	1.89318000	4.51446200	-0.61322900
C	4.46619700	0.20055200	-0.76305300
H	3.41044500	0.05559900	-0.53065900
C	-1.30779600	4.60222300	-3.36165100
H	-0.39702100	4.42134600	-3.93853200
H	-2.15480800	4.59679400	-4.05542800
H	-1.24514600	5.60613000	-2.92794100
C	-2.72982700	3.81620000	-1.39626000
H	-3.63669900	3.79384500	-2.01089900
H	-2.82552900	3.05621400	-0.61759000
H	-2.66907400	4.80295600	-0.92348800
C	2.80777200	5.80020600	-2.05027100
H	3.72976000	6.36946900	-2.21001800
H	2.69264300	5.09608400	-2.87713900
H	1.96859000	6.50250500	-2.08040900
C	2.91359200	6.03700400	0.47969100
H	2.90194400	5.50626800	1.43510500
H	3.82121500	6.64825900	0.44404400
H	2.05592000	6.71651200	0.46197500
C	5.27381600	-0.60421700	0.26965500
H	6.34909500	-0.57515400	0.06621600

H	5.11144800	-0.22612700	1.28253200
H	4.96543200	-1.65388200	0.24861600
C	4.69685600	-0.32801400	-2.19195700
H	4.06190200	0.20544800	-2.90238500
H	5.74168400	-0.19847000	-2.49491000
H	4.45641600	-1.39455100	-2.24997000
C	0.92129200	-2.10022200	-3.22057000
H	0.23434000	-2.64685300	-3.87475000
H	1.53740200	-1.44890900	-3.84603100
H	1.57643500	-2.83797700	-2.74492500
C	-0.67204100	-2.20228700	-1.23415600
H	-1.20189900	-1.60607900	-0.48796900
H	-1.41392900	-2.76346100	-1.81359400
H	-0.02915400	-2.92625900	-0.72092300
C	-0.84324700	1.14988900	0.89157400
O	-1.86854300	0.77584000	0.27719100
O	-0.63063300	1.26785700	2.11630800

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C	0.31119700	1.47727300	-0.00945400
C	1.56211200	1.91052200	0.34689100
C	1.61880400	1.92831400	-1.88908800
N	0.41432800	1.51101400	-1.43617500
H	1.99922200	2.06201900	1.32149600
N	2.35698200	2.18602700	-0.80010600
C	3.71822900	2.64457400	-0.79212500
C	4.75640200	1.69328900	-0.76261200
C	3.97336400	4.02914900	-0.77089200
C	6.07231000	2.16395000	-0.72604700
C	5.30741200	4.44637300	-0.73341200
C	6.34881000	3.52609400	-0.71348400
H	6.89109000	1.45263800	-0.71434900
H	5.53212200	5.50743500	-0.72751400
H	7.37778800	3.87099900	-0.69129600
C	-0.66853000	1.13892100	-2.30801300
C	-1.59415100	2.12079400	-2.70382300
C	-0.78872800	-0.20234200	-2.71321800
C	-2.64986800	1.73016200	-3.53349800
C	-1.86262200	-0.54309800	-3.54133900
C	-2.78519900	0.41182500	-3.95190300
H	-3.37443300	2.46971300	-3.85727200
H	-1.97503100	-1.57041100	-3.87121100
H	-3.60950800	0.12855000	-4.59917800
C	-1.48788800	3.56999700	-2.24561300
H	-0.60068800	3.65121100	-1.61791200
C	0.19192200	-1.27866600	-2.26485200
H	0.96250600	-0.79306100	-1.66679300
C	2.85519600	5.06508800	-0.78983600

H	1.90670200	4.52753400	-0.80633000
C	4.48743000	0.19296700	-0.77204500
H	3.40641700	0.05122200	-0.77568600
C	-1.29931100	4.53167300	-3.43253800
H	-0.39420500	4.27641300	-3.98742500
H	-2.15566000	4.50280800	-4.11538300
H	-1.19974600	5.56081900	-3.06984500
C	-2.69270600	3.96522700	-1.37152600
H	-3.63124300	3.92017700	-1.93450200
H	-2.77769300	3.30068700	-0.50833900
H	-2.57363400	4.99023800	-1.00416000
C	2.90937300	5.93157100	-2.06135500
H	3.84495600	6.49867800	-2.11989700
H	2.81215800	5.30411200	-2.94935500
H	2.08321400	6.65064500	-2.05843600
C	2.86883900	5.92877100	0.48568000
H	2.79124700	5.31086200	1.38448500
H	3.78612200	6.52202300	0.56158900
H	2.02288800	6.62343300	0.47909900
C	5.03138200	-0.48382900	0.50050900
H	6.12179600	-0.40654800	0.56486500
H	4.60754500	-0.03329900	1.40216100
H	4.77298700	-1.54749900	0.50068800
C	5.03901800	-0.47278800	-2.04632800
H	4.56918100	-0.04187900	-2.93257400
H	6.12577800	-0.35529700	-2.12093300
H	4.82002100	-1.54585900	-2.03158500
C	0.89496700	-1.94616800	-3.45988300
H	0.18231600	-2.46464700	-4.11091200
H	1.43464500	-1.19875600	-4.04486800
H	1.61743900	-2.68880400	-3.10330800
C	-0.49871700	-2.31036200	-1.35320000
H	-0.94731400	-1.81973400	-0.48607700
H	-1.28543300	-2.85562200	-1.88603700
H	0.22972600	-3.04451800	-0.99219100
C	2.08525900	2.08451000	-3.35254700
O	2.57634900	1.05124100	-3.84606400
O	1.90806600	3.22216600	-3.82912800

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C	0.38506600	1.50906200	-0.00424100
C	1.61862300	1.93403100	0.37042300
C	1.60121600	1.92085400	-1.86237200
N	0.39976100	1.50825000	-1.41484000
H	2.01518700	2.07347600	1.35971000
N	2.36223100	2.18589400	-0.78159400
C	3.73073400	2.64638000	-0.80446600
C	4.76269500	1.69027600	-0.79884600

C	3.97795300	4.03103600	-0.80545200
C	6.07835000	2.16299000	-0.79738200
C	5.31297500	4.44658300	-0.80314900
C	6.35290700	3.52509600	-0.79998600
H	6.89735400	1.45262700	-0.79993900
H	5.53837800	5.50697400	-0.81003700
H	7.38182500	3.86992400	-0.80304600
C	-0.67726500	1.13771000	-2.31672200
C	-1.56428200	2.13499400	-2.74795900
C	-0.75939600	-0.19316500	-2.75245100
C	-2.54476900	1.76791700	-3.67316400
C	-1.75747100	-0.50649900	-3.67804500
C	-2.63828900	0.46315900	-4.14083700
H	-3.24725300	2.51424600	-4.02644400
H	-1.84788100	-1.52594300	-4.03552300
H	-3.40544800	0.19911300	-4.86173600
C	-1.52946400	3.55757700	-2.20581300
H	-0.65929700	3.64725200	-1.55351200
C	0.14392000	-1.29276000	-2.21120700
H	0.89405100	-0.82656400	-1.57035600
C	2.86212400	5.06982900	-0.80420900
H	1.90895600	4.54058900	-0.82709200
C	4.49868900	0.18897400	-0.79123900
H	3.41903300	0.03614500	-0.80020500
C	-1.36266600	4.60256000	-3.32263100
H	-0.44730700	4.41692100	-3.88840100
H	-2.21223300	4.59175200	-4.01322800
H	-1.30475300	5.60694000	-2.88938200
C	-2.77290800	3.82971700	-1.33596500
H	-3.68673500	3.81397300	-1.93945700
H	-2.86778200	3.07459700	-0.55246200
H	-2.69866300	4.81726200	-0.86794900
C	2.91280100	5.95551700	-2.06253500
H	3.84488700	6.52813900	-2.11253700
H	2.81846600	5.34336500	-2.96110800
H	2.08359400	6.66996600	-2.04709400
C	2.88629700	5.91324400	0.48490100
H	2.80870800	5.28485700	1.37620200
H	3.80816700	6.49819200	0.56397400
H	2.04528800	6.61303800	0.49198700
C	5.04159800	-0.46825100	0.49221600
H	6.13079800	-0.38121100	0.55814200
H	4.61256800	-0.01197900	1.38832700
H	4.79112100	-1.53320600	0.50354600
C	5.05829600	-0.48931100	-2.05534200
H	4.59845100	-0.06479700	-2.94947600
H	6.14563000	-0.37732600	-2.12189000
H	4.83468700	-1.56064900	-2.03200400
C	0.90555400	-2.02648900	-3.32878700

H	0.22206600	-2.54661900	-4.00807000
H	1.50951900	-1.32339000	-3.90608000
H	1.57126400	-2.78001400	-2.89424800
C	-0.66572500	-2.26146200	-1.32622200
H	-1.19501500	-1.71503800	-0.54241400
H	-1.40446000	-2.81187400	-1.91881300
H	0.00135300	-2.99446100	-0.85964000
C	2.06500900	2.07842500	-3.33297400
O	2.57092800	1.04904000	-3.80824400
O	1.87754700	3.21651700	-3.79301700
C	-0.78515200	1.10815800	0.91856300
O	-1.82063200	0.72634300	0.33822900
O	-0.50900500	1.22862600	2.12743200

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C	0.38029900	1.51007900	-0.00401700
C	1.62121200	1.93418200	0.38134600
C	1.60074300	1.92007000	-1.82370800
N	0.39846600	1.51161200	-1.40146000
H	2.00983000	2.07012600	1.37491500
N	2.36853400	2.18511100	-0.75790200
C	3.74173000	2.64699200	-0.80339200
C	4.76957200	1.68655000	-0.80422800
C	3.98267300	4.03263900	-0.81973000
C	6.08398700	2.16079000	-0.84189500
C	5.31770900	4.44620600	-0.85632700
C	6.35637300	3.52321100	-0.86958600
H	6.90469500	1.45318900	-0.84536500
H	5.54580700	5.50544100	-0.87098000
H	7.38411800	3.86763000	-0.89700700
C	-0.66092700	1.14738000	-2.33566800
C	-1.53404000	2.15317400	-2.77722600
C	-0.72240500	-0.18013000	-2.78630900
C	-2.47219100	1.79792300	-3.75007200
C	-1.68023800	-0.47685600	-3.75944500
C	-2.53950200	0.50128500	-4.24453900
H	-3.16934100	2.54371300	-4.11305000
H	-1.76462500	-1.49170700	-4.12961300
H	-3.27707100	0.24752900	-4.99784300
C	-1.54701600	3.55654200	-2.18434100
H	-0.68311000	3.65650500	-1.52279000
C	0.13760400	-1.29313500	-2.20086400
H	0.88263600	-0.84014200	-1.54234100
C	2.86588800	5.07077000	-0.79075600
H	1.90967800	4.54441900	-0.76588500
C	4.50408300	0.18570700	-0.75847000
H	3.42418100	0.03028400	-0.72007800
C	-1.42907200	4.65390800	-3.25647700

H	-0.52830700	4.53078200	-3.86511200
H	-2.28888300	4.65281100	-3.93172700
H	-1.38783600	5.63924200	-2.78330300
C	-2.80281700	3.75027400	-1.30977900
H	-3.71090600	3.72275800	-1.91972000
H	-2.87271200	2.96293500	-0.55682300
H	-2.76657700	4.72084200	-0.80567600
C	2.87419200	5.94616100	-2.05804800
H	3.79034800	6.53867200	-2.12995700
H	2.79743100	5.34040000	-2.96490400
H	2.02992200	6.64050600	-2.04254000
C	2.93550500	5.93506000	0.48261900
H	2.89282600	5.32039000	1.38483700
H	3.85755800	6.52184200	0.51815000
H	2.09437300	6.63280900	0.51044000
C	5.09368300	-0.45140900	0.51432500
H	6.18361400	-0.36572500	0.53784900
H	4.69955800	0.02179000	1.41671600
H	4.84194000	-1.51447800	0.55425200
C	5.02472100	-0.51977800	-2.02496700
H	4.58579200	-0.09416000	-2.93124500
H	6.11166300	-0.43746500	-2.11125100
H	4.77340200	-1.58332700	-1.99502800
C	0.90302500	-2.08175600	-3.27804500
H	0.22356800	-2.61323900	-3.94971700
H	1.53094300	-1.42755300	-3.89009400
H	1.54751600	-2.83029900	-2.80825300
C	-0.72659300	-2.22329000	-1.32485800
H	-1.26086100	-1.65017700	-0.56465000
H	-1.46383400	-2.75608500	-1.93315700
H	-0.09716700	-2.96927800	-0.83015100
C	-0.81019700	1.10560700	0.90596700
O	-1.82821100	0.74202300	0.29086200
O	-0.53452400	1.21666100	2.10906500
H	1.90297500	2.02068200	-2.85202800

8. X-Ray Crystal Data for Carboxylate 5a

The compound **5a** crystallizes as colorless block-like crystals from a dichloromethane/hexanes/water solution. There are four molecules of the compound, two water molecules and four, partial occupancy dichloromethane molecules of crystallization in the asymmetric unit of the primitive, acentric, orthorhombic space group $Pna2_1$ (Figure 1). Although there are four crystallographically independent molecules of the diazole, they are chemically identical. Examination of the data for a super- or sub-lattice did not reveal either a larger or smaller cell. The structure refines with a racemic twin component of ~9%, indicative of a chiral space group, rather than a centrosymmetric space group.[5] If the twin percentage were ~50% there would be reason to consider a centrosymmetric space group. The structure refines well in this acentric space group.

The diazole appears to be the Zwitterion as predicted. There is no evidence for the presence of hydrogen atoms on the carboxylate functionality. However, this may also have been due to the slightly weak diffraction due to disorder and partial occupancy solvent (see below). The four independent diazoles are essentially identical, and differ in torsion angles and the amount of thermal motion exhibited in the peripheral atoms (^{i}Pr predominantly). The derived metrics (bond distances and angles) within these molecules are as expected.

The solvent molecules of crystallization exhibit disorder and partial occupancy within the lattice. All four dichloromethane molecules were modeled with a refined occupancy yielding 0.92, 0.95, 0.20 and 0.19. These variable amounts of dichloromethane were reflected in the data, which exhibited a drop-off in intensity at high resolution. The two water molecules were located and presumed to be water since they are relatively close (within H-bonding contact) of H-bond acceptor atoms, and are located in voids, which could not contain any other species. Due to the disorder and weak diffraction, the hydrogen atoms on these water molecules could not be located but have been included in the chemical formula for completeness.

An arbitrary sphere of data were collected on a colorless block-like crystal, having approximate dimensions of 0.15 × 0.14 × 0.06 mm, on a Bruker APEX-II diffractometer using a combination of ω- and φ-scans of 0.5°.[6] Data were corrected for absorption and polarization effects and analyzed for space group determination. The structure was solved by direct methods and expanded routinely.[7] The model was refined by full-matrix least-squares analysis of F^2 against all reflections. All non-hydrogen atoms were refined with anisotropic thermal displacement parameters. Unless otherwise noted, hydrogen atoms were included in calculated positions. Thermal parameters for the hydrogens were tied to the isotropic thermal parameter of the atom to which they are bonded (1.5 × for methyl, 1.2 × for all others).

Figure 1. Asymmetric unit cell of **5a**

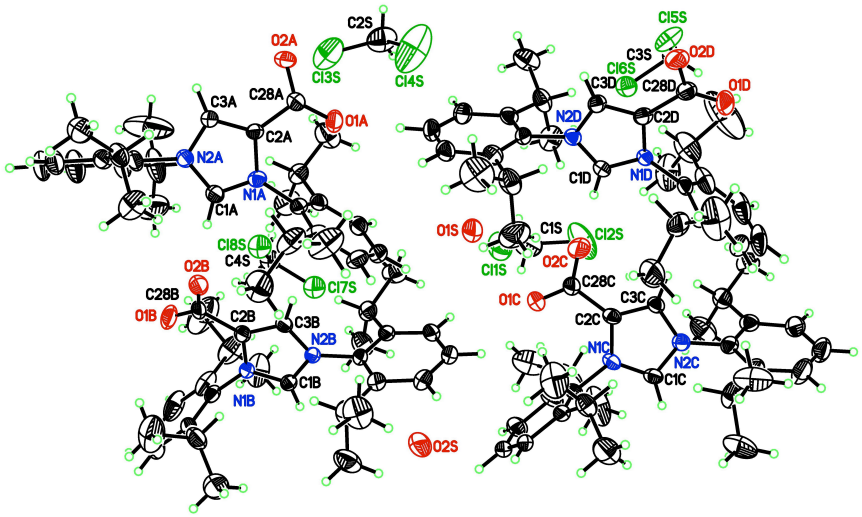

Table 1. Crystal data and structure refinement for 5a.

Empirical formula	$C_{114.27}H_{156.53}Cl_{4.53}N_8O_{10}$
Formula weight	1962.89
Temperature	120(2) K
Wavelength	1.54184 Å
Crystal system	Orthorhombic
Space group	$Pna2_1$
Unit cell dimensions	a = 25.8365(6) Å α = 90°
	b = 10.6650(3) Å β = 90°
	c = 41.6219(9) Å γ = 90°
Volume	11468.8(5) $Å^3$
Z	4
Density (calculated)	1.137 $g.cm^{-3}$
Absorption coefficient (μ)	1.503 mm^{-1}
F(000)	4221
Crystal color, habit	colorless, block
Crystal size	0.15 × 0.14 × 0.06 mm^3
θ range for data collection	2.12 to 71.66°
Index ranges	$-29 \le h \le 31$, $-13 \le k \le 13$, $-51 \le l \le 50$
Reflections collected	289546
Independent reflections	21924 [R_{int} = 0.0657]
Completeness to θ = 71.66°	99.3 %
Absorption correction	Numerical
Max. and min. transmission	1.0000 and 0.9312
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	21924 / 1 / 1295
Goodness-of-fit on F^2	1.035
Final R indices [I>2σ(I)]	R_1 = 0.0569, wR_2 = 0.1494
R indices (all data)	R_1 = 0.0616, wR_2 = 0.1546
Absolute structure parameter	0.000(16)
Largest diff. peak and hole	0.748 and -0.589 $e^-.Å^{-3}$

Table 2. Atomic coordinates and equivalent isotropic displacement parameters (Å^2) for 5a. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
O(1A)	0.99064(8)	0.1256(2)	0.16136(5)	0.044(1)
O(2A)	1.05868(8)	0.1189(3)	0.19394(5)	0.053(1)
N(1A)	0.92323(8)	0.12813(18)	0.21694(5)	0.026(1)
N(2A)	0.94684(8)	0.10798(19)	0.26650(5)	0.027(1)
C(1A)	0.90603(10)	0.1180(2)	0.24684(6)	0.027(1)
C(2A)	0.97735(9)	0.1252(2)	0.21722(6)	0.024(1)
C(3A)	0.99155(9)	0.1134(2)	0.24822(6)	0.025(1)
C(4A)	0.89032(9)	0.1562(2)	0.18956(6)	0.026(1)
C(5A)	0.86904(11)	0.0573(3)	0.17246(7)	0.036(1)
C(6A)	0.83858(11)	0.0886(3)	0.14562(7)	0.037(1)
C(7A)	0.83158(10)	0.2119(3)	0.13653(7)	0.035(1)
C(8A)	0.85303(10)	0.3072(3)	0.15468(7)	0.032(1)
C(9A)	0.88256(10)	0.2818(2)	0.18192(6)	0.028(1)
C(10A)	0.87596(15)	-0.0776(3)	0.18254(10)	0.054(1)
C(11A)	0.88419(18)	-0.1652(3)	0.15419(12)	0.069(1)
C(12A)	0.8297(2)	-0.1215(4)	0.20308(11)	0.073(1)
C(13A)	0.90472(11)	0.3885(2)	0.20203(7)	0.034(1)
C(14A)	0.94406(16)	0.4652(3)	0.18366(10)	0.059(1)
C(15A)	0.86134(15)	0.4704(4)	0.21557(10)	0.058(1)
C(16A)	0.94396(10)	0.0975(3)	0.30133(6)	0.032(1)
C(17A)	0.92957(15)	0.2016(3)	0.31896(8)	0.047(1)
C(18A)	0.92738(17)	0.1862(3)	0.35234(8)	0.058(1)
C(19A)	0.93823(16)	0.0725(4)	0.36668(8)	0.056(1)
C(20A)	0.95264(12)	-0.0288(3)	0.34836(8)	0.044(1)
C(21A)	0.95612(10)	-0.0194(3)	0.31507(7)	0.033(1)
C(22A)	0.91662(18)	0.3282(3)	0.30398(8)	0.061(1)
C(23A)	0.95233(18)	0.4309(5)	0.3155(2)	0.140(4)
C(24A)	0.86259(17)	0.3666(4)	0.31071(15)	0.081(2)
C(25A)	0.97172(12)	-0.1315(3)	0.29467(7)	0.037(1)
C(26A)	1.00643(13)	-0.2248(3)	0.31268(9)	0.047(1)
C(27A)	0.92434(16)	-0.1989(3)	0.28161(10)	0.059(1)
C(28A)	1.01170(10)	0.1261(3)	0.18777(6)	0.031(1)
O(1B)	0.74330(9)	0.2506(3)	0.29364(5)	0.056(1)
O(2B)	0.79726(8)	0.1366(2)	0.26262(5)	0.047(1)
N(1B)	0.67718(8)	0.28026(18)	0.23884(5)	0.024(1)
N(2B)	0.69997(8)	0.27169(19)	0.18899(5)	0.024(1)
C(1B)	0.66102(9)	0.2994(2)	0.20887(6)	0.024(1)
C(2B)	0.72760(9)	0.2365(2)	0.23835(6)	0.028(1)
C(3B)	0.74156(9)	0.2308(2)	0.20705(6)	0.029(1)
C(4B)	0.64375(10)	0.2975(3)	0.26665(6)	0.028(1)
C(5B)	0.61789(10)	0.1924(3)	0.27839(6)	0.036(1)
C(6B)	0.58555(12)	0.2131(4)	0.30517(7)	0.055(1)
C(7B)	0.58035(14)	0.3302(5)	0.31844(8)	0.066(1)
C(8B)	0.60682(17)	0.4314(4)	0.30596(9)	0.063(1)

C(9B)	0.63909(13)	0.4176(3)	0.27968(8)	0.046(1)
C(10B)	0.62363(14)	0.0633(3)	0.26375(8)	0.047(1)
C(11B)	0.6417(3)	-0.0307(4)	0.28945(12)	0.087(2)
C(12B)	0.5730(2)	0.0214(5)	0.24806(11)	0.084(2)
C(13B)	0.66781(18)	0.5285(3)	0.26627(11)	0.064(1)
C(14B)	0.7027(3)	0.5901(6)	0.29144(17)	0.130(3)
C(15B)	0.6295(2)	0.6213(4)	0.25162(11)	0.076(1)
C(16B)	0.69880(9)	0.2776(2)	0.15418(6)	0.026(1)
C(17B)	0.71421(9)	0.3897(2)	0.13933(6)	0.029(1)
C(18B)	0.71690(10)	0.3880(3)	0.10589(7)	0.037(1)
C(19B)	0.70459(11)	0.2820(3)	0.08884(7)	0.039(1)
C(20B)	0.68837(12)	0.1737(3)	0.10424(7)	0.039(1)
C(21B)	0.68481(10)	0.1699(3)	0.13752(6)	0.032(1)
C(22B)	0.72572(11)	0.5076(3)	0.15854(7)	0.036(1)
C(23B)	0.76316(13)	0.5980(3)	0.14172(9)	0.049(1)
C(24B)	0.67498(14)	0.5762(3)	0.16632(9)	0.049(1)
C(25B)	0.66309(14)	0.0559(3)	0.15444(8)	0.044(1)
C(26B)	0.6822(2)	-0.0687(3)	0.14005(11)	0.069(1)
C(27B)	0.60388(15)	0.0627(4)	0.15453(10)	0.062(1)
C(28B)	0.75905(10)	0.2053(3)	0.26806(7)	0.038(1)
O(1C)	0.75609(8)	0.4121(2)	0.02946(5)	0.043(1)
O(2C)	0.82454(8)	0.3856(3)	-0.00199(6)	0.062(1)
N(1C)	0.69009(8)	0.37803(19)	-0.02638(5)	0.028(1)
N(2C)	0.71430(8)	0.39375(19)	-0.07603(5)	0.028(1)
C(1C)	0.67326(9)	0.3834(2)	-0.05657(6)	0.029(1)
C(2C)	0.74423(9)	0.3850(2)	-0.02608(6)	0.027(1)
C(3C)	0.75850(9)	0.3942(2)	-0.05747(6)	0.027(1)
C(4C)	0.65617(9)	0.3456(2)	0.00026(6)	0.029(1)
C(5C)	0.63339(11)	0.4418(3)	0.01830(8)	0.039(1)
C(6C)	0.60085(11)	0.4052(3)	0.04330(8)	0.041(1)
C(7C)	0.59159(10)	0.2811(3)	0.04993(7)	0.036(1)
C(8C)	0.61469(10)	0.1890(3)	0.03175(6)	0.032(1)
C(9C)	0.64786(9)	0.2187(2)	0.00627(6)	0.029(1)
C(10C)	0.64212(16)	0.5779(3)	0.00967(11)	0.064(1)
C(11C)	0.5986(3)	0.6249(4)	-0.01268(12)	0.088(2)
C(12C)	0.64654(17)	0.6600(4)	0.04030(14)	0.077(1)
C(13C)	0.67366(12)	0.1153(3)	-0.01299(7)	0.038(1)
C(14C)	0.63374(18)	0.0296(4)	-0.02879(10)	0.065(1)
C(15C)	0.71178(19)	0.0436(4)	0.00785(11)	0.074(1)
C(16C)	0.71149(10)	0.4050(2)	-0.11071(6)	0.030(1)
C(17C)	0.69722(13)	0.2985(3)	-0.12861(7)	0.041(1)
C(18C)	0.69506(16)	0.3125(3)	-0.16187(8)	0.054(1)
C(19C)	0.70630(14)	0.4263(3)	-0.17628(8)	0.051(1)
C(20C)	0.72041(12)	0.5285(3)	-0.15797(7)	0.041(1)
C(21C)	0.72412(10)	0.5211(3)	-0.12470(7)	0.033(1)
C(22C)	0.68411(15)	0.1736(3)	-0.11327(8)	0.052(1)
C(23C)	0.62837(15)	0.1383(4)	-0.11989(13)	0.070(1)
C(24C)	0.71820(16)	0.0653(4)	-0.12711(15)	0.079(1)
C(25C)	0.73938(12)	0.6334(3)	-0.10458(7)	0.037(1)

C(26C)	0.69143(16)	0.6990(3)	-0.09080(11)	0.061(1)
C(27C)	0.77303(13)	0.7276(3)	-0.12298(9)	0.046(1)
C(28C)	0.77804(10)	0.3933(3)	0.00335(6)	0.032(1)
O(1D)	1.00865(9)	0.2476(3)	-0.10329(5)	0.058(1)
O(2D)	1.06340(8)	0.1392(2)	-0.07098(5)	0.049(1)
N(1D)	0.94225(8)	0.28471(18)	-0.04899(5)	0.024(1)
N(2D)	0.96438(8)	0.27914(18)	0.00102(5)	0.024(1)
C(1D)	0.92630(9)	0.3068(2)	-0.01901(6)	0.024(1)
C(2D)	0.99277(9)	0.2391(2)	-0.04800(6)	0.029(1)
C(3D)	1.00602(10)	0.2358(2)	-0.01648(6)	0.029(1)
C(4D)	0.90932(9)	0.3001(2)	-0.07699(6)	0.029(1)
C(5D)	0.90419(14)	0.4191(3)	-0.09035(8)	0.048(1)
C(6D)	0.87173(17)	0.4323(5)	-0.11642(9)	0.064(1)
C(7D)	0.84564(16)	0.3305(5)	-0.12900(8)	0.072(2)
C(8D)	0.85196(13)	0.2137(4)	-0.11549(8)	0.056(1)
C(9D)	0.88363(11)	0.1953(3)	-0.08876(7)	0.036(1)
C(10D)	0.93211(18)	0.5329(3)	-0.07690(11)	0.064(1)
C(11D)	0.8931(2)	0.6253(4)	-0.06250(11)	0.081(2)
C(12D)	0.9657(4)	0.5921(6)	-0.1027(2)	0.155(4)
C(13D)	0.88990(14)	0.0669(3)	-0.07427(8)	0.049(1)
C(14D)	0.8396(2)	0.0234(6)	-0.05793(11)	0.087(2)
C(15D)	0.9073(3)	-0.0270(4)	-0.09921(12)	0.093(2)
C(16D)	0.96322(9)	0.2923(2)	0.03583(6)	0.025(1)
C(17D)	0.95061(10)	0.1868(2)	0.05398(7)	0.032(1)
C(18D)	0.95304(11)	0.2005(3)	0.08739(7)	0.036(1)
C(19D)	0.96613(12)	0.3141(3)	0.10122(7)	0.039(1)
C(20D)	0.97726(11)	0.4159(3)	0.08243(7)	0.037(1)
C(21D)	0.97597(10)	0.4089(2)	0.04894(6)	0.028(1)
C(22D)	0.93310(14)	0.0655(3)	0.03886(8)	0.047(1)
C(23D)	0.87356(18)	0.0670(4)	0.03589(12)	0.075(1)
C(24D)	0.9515(2)	-0.0505(3)	0.05751(13)	0.075(1)
C(25D)	0.98530(12)	0.5235(3)	0.02800(7)	0.039(1)
C(26D)	0.93432(14)	0.5939(3)	0.02345(9)	0.049(1)
C(27D)	1.02605(13)	0.6131(3)	0.04173(9)	0.050(1)
C(28D)	1.02430(10)	0.2048(3)	-0.07728(7)	0.038(1)
O(1S)	0.83688(9)	0.4355(2)	0.07675(6)	0.051(1)
O(2S)	0.57010(11)	0.4274(3)	0.11713(6)	0.071(1)
C(1S)	0.79339(18)	0.6963(4)	0.04280(13)	0.068(1)
Cl(1S)	0.77532(5)	0.82395(11)	0.06776(3)	0.075(1)
Cl(2S)	0.79433(7)	0.73711(11)	0.00235(4)	0.091(1)
C(2S)	1.03197(19)	0.8392(4)	0.15881(12)	0.071(1)
Cl(3S)	1.01777(6)	0.77941(11)	0.19768(4)	0.094(1)
Cl(4S)	1.02938(10)	0.72391(16)	0.12984(5)	0.141(1)
C(3S)	1.0161(6)	0.8516(13)	-0.0620(3)	0.036(3)
Cl(5S)	1.04629(16)	0.7013(3)	-0.06071(11)	0.054(1)
Cl(6S)	0.97581(14)	0.8716(3)	-0.02787(9)	0.043(1)
C(4S)	0.7466(7)	0.8418(16)	0.2520(4)	0.045(4)
Cl(7S)	0.70979(18)	0.8642(4)	0.21803(11)	0.053(1)
Cl(8S)	0.78078(18)	0.6964(4)	0.25137(12)	0.056(1)

H(1A)	0.8707	0.1178	0.2532	0.033
H(3A)	1.0260	0.1095	0.2561	0.030
H(6A)	0.8225	0.0237	0.1335	0.045
H(7A)	0.8121	0.2312	0.1178	0.042
H(8A)	0.8475	0.3919	0.1484	0.039
H(10A)	0.9076	-0.0820	0.1963	0.065
H(11A)	0.9125	-0.1335	0.1408	0.104
H(11B)	0.8524	-0.1694	0.1414	0.104
H(11C)	0.8929	-0.2491	0.1621	0.104
H(12A)	0.7978	-0.1158	0.1904	0.109
H(12B)	0.8267	-0.0680	0.2221	0.109
H(12C)	0.8352	-0.2086	0.2098	0.109
H(13A)	0.9231	0.3498	0.2207	0.041
H(14A)	0.9273	0.5047	0.1651	0.088
H(14B)	0.9720	0.4104	0.1762	0.088
H(14C)	0.9584	0.5301	0.1978	0.088
H(15A)	0.8357	0.4173	0.2263	0.086
H(15B)	0.8447	0.5166	0.1980	0.086
H(15C)	0.8758	0.5300	0.2311	0.086
H(18A)	0.9182	0.2557	0.3654	0.070
H(19A)	0.9357	0.0642	0.3893	0.067
H(20A)	0.9603	-0.1063	0.3585	0.053
H(22A)	0.9207	0.3206	0.2802	0.073
H(23A)	0.9883	0.4075	0.3111	0.211
H(23B)	0.9478	0.4426	0.3387	0.211
H(23C)	0.9441	0.5093	0.3044	0.211
H(24A)	0.8587	0.3842	0.3337	0.122
H(24B)	0.8390	0.2988	0.3046	0.122
H(24C)	0.8543	0.4422	0.2983	0.122
H(25A)	0.9918	-0.0991	0.2759	0.045
H(26A)	0.9869	-0.2625	0.3304	0.071
H(26B)	1.0367	-0.1808	0.3212	0.071
H(26C)	1.0178	-0.2908	0.2979	0.071
H(27A)	0.9029	-0.1396	0.2695	0.089
H(27B)	0.9042	-0.2335	0.2995	0.089
H(27C)	0.9353	-0.2671	0.2674	0.089
H(1B)	0.6276	0.3278	0.2027	0.029
H(3B)	0.7741	0.2036	0.1990	0.034
H(6B)	0.5670	0.1447	0.3142	0.066
H(7B)	0.5582	0.3417	0.3364	0.079
H(8B)	0.6028	0.5116	0.3155	0.075
H(10B)	0.6508	0.0678	0.2467	0.057
H(11D)	0.6737	-0.0003	0.2994	0.130
H(11E)	0.6481	-0.1124	0.2794	0.130
H(11F)	0.6149	-0.0394	0.3059	0.130
H(12D)	0.5464	0.0111	0.2646	0.126
H(12E)	0.5784	-0.0586	0.2370	0.126
H(12F)	0.5618	0.0849	0.2325	0.126
H(13B)	0.6905	0.4973	0.2485	0.077

H(14D)	0.6819	0.6155	0.3100	0.194
H(14E)	0.7195	0.6640	0.2821	0.194
H(14F)	0.7292	0.5301	0.2984	0.194
H(15D)	0.6093	0.5792	0.2349	0.114
H(15E)	0.6485	0.6918	0.2422	0.114
H(15F)	0.6062	0.6524	0.2684	0.114
H(18B)	0.7274	0.4614	0.0947	0.045
H(19B)	0.7072	0.2829	0.0661	0.046
H(20B)	0.6796	0.1017	0.0920	0.047
H(22B)	0.7419	0.4815	0.1793	0.044
H(23D)	0.7935	0.5515	0.1341	0.074
H(23E)	0.7742	0.6629	0.1569	0.074
H(23F)	0.7457	0.6374	0.1234	0.074
H(24D)	0.6590	0.6056	0.1463	0.073
H(24E)	0.6823	0.6480	0.1803	0.073
H(24F)	0.6513	0.5186	0.1773	0.073
H(25B)	0.6749	0.0591	0.1773	0.053
H(26D)	0.6673	-0.0798	0.1186	0.104
H(26E)	0.6714	-0.1383	0.1539	0.104
H(26F)	0.7201	-0.0674	0.1385	0.104
H(27D)	0.5928	0.1413	0.1646	0.092
H(27E)	0.5899	-0.0084	0.1666	0.092
H(27F)	0.5911	0.0597	0.1324	0.092
H(1C)	0.6381	0.3804	-0.0632	0.035
H(3C)	0.7930	0.4000	-0.0652	0.032
H(6C)	0.5846	0.4677	0.0561	0.049
H(7C)	0.5692	0.2587	0.0671	0.044
H(8C)	0.6080	0.1035	0.0366	0.039
H(10C)	0.6756	0.5839	-0.0023	0.077
H(11G)	0.5968	0.5711	-0.0318	0.132
H(11H)	0.6059	0.7113	-0.0193	0.132
H(11I)	0.5654	0.6219	-0.0013	0.132
H(11X)	0.5819	0.6984	-0.0031	0.132
H(11Y)	0.5728	0.5582	-0.0156	0.132
H(11Z)	0.6133	0.6476	-0.0336	0.132
H(12G)	0.6131	0.6620	0.0514	0.115
H(12H)	0.6565	0.7455	0.0342	0.115
H(12I)	0.6728	0.6245	0.0546	0.115
H(13C)	0.6939	0.1563	-0.0306	0.046
H(14G)	0.6138	-0.0138	-0.0121	0.098
H(14H)	0.6515	-0.0322	-0.0423	0.098
H(14I)	0.6103	0.0798	-0.0421	0.098
H(15G)	0.7362	0.1025	0.0177	0.111
H(15H)	0.7308	-0.0166	-0.0054	0.111
H(15I)	0.6929	-0.0013	0.0247	0.111
H(18C)	0.6857	0.2429	-0.1749	0.065
H(19C)	0.7043	0.4340	-0.1990	0.061
H(20C)	0.7278	0.6059	-0.1683	0.049
H(22C)	0.6896	0.1795	-0.0895	0.062

H(23G)	0.6055	0.2059	-0.1126	0.105
H(23H)	0.6199	0.0609	-0.1084	0.105
H(23I)	0.6236	0.1254	-0.1430	0.105
H(24G)	0.7148	0.0632	-0.1506	0.118
H(24H)	0.7066	-0.0150	-0.1181	0.118
H(24I)	0.7545	0.0795	-0.1213	0.118
H(25C)	0.7602	0.6017	-0.0860	0.045
H(26G)	0.6697	0.7293	-0.1085	0.092
H(26H)	0.7023	0.7700	-0.0775	0.092
H(26I)	0.6717	0.6395	-0.0777	0.092
H(27G)	0.8023	0.6836	-0.1328	0.069
H(27H)	0.7860	0.7914	-0.1081	0.069
H(27I)	0.7523	0.7679	-0.1398	0.069
H(1D)	0.8931	0.3373	-0.0131	0.029
H(3D)	1.0382	0.2085	-0.0080	0.034
H(6D)	0.8672	0.5126	-0.1259	0.077
H(7D)	0.8234	0.3411	-0.1469	0.086
H(8D)	0.8344	0.1440	-0.1246	0.067
H(10D)	0.9553	0.5037	-0.0592	0.077
H(11J)	0.8735	0.5837	-0.0454	0.121
H(11K)	0.8693	0.6538	-0.0793	0.121
H(11L)	0.9116	0.6976	-0.0536	0.121
H(12J)	0.9439	0.6205	-0.1205	0.232
H(12K)	0.9907	0.5302	-0.1106	0.232
H(12L)	0.9844	0.6640	-0.0936	0.232
H(13D)	0.9174	0.0721	-0.0574	0.059
H(14J)	0.8128	0.0106	-0.0742	0.131
H(14K)	0.8281	0.0874	-0.0426	0.131
H(14L)	0.8459	-0.0556	-0.0465	0.131
H(15J)	0.9368	0.0070	-0.1111	0.139
H(15K)	0.8787	-0.0438	-0.1141	0.139
H(15L)	0.9175	-0.1051	-0.0886	0.139
H(18D)	0.9456	0.1306	0.1008	0.043
H(19D)	0.9674	0.3215	0.1240	0.047
H(20D)	0.9861	0.4932	0.0924	0.044
H(22D)	0.9480	0.0611	0.0167	0.056
H(23J)	0.8628	0.1402	0.0233	0.113
H(23K)	0.8581	0.0712	0.0574	0.113
H(23L)	0.8619	-0.0096	0.0251	0.113
H(24J)	0.9343	-0.0532	0.0785	0.113
H(24K)	0.9890	-0.0460	0.0606	0.113
H(24L)	0.9429	-0.1263	0.0453	0.113
H(25D)	0.9975	0.4942	0.0065	0.047
H(26J)	0.9228	0.6278	0.0441	0.074
H(26K)	0.9080	0.5363	0.0151	0.074
H(26L)	0.9394	0.6628	0.0082	0.074
H(27J)	1.0573	0.5659	0.0473	0.075
H(27K)	1.0123	0.6538	0.0611	0.075
H(27L)	1.0345	0.6771	0.0257	0.075

H(1SA)	0.8282	0.6664	0.0492	0.081
H(1SB)	0.7687	0.6265	0.0460	0.081
H(2SA)	1.0068	0.9061	0.1534	0.085
H(2SB)	1.0670	0.8770	0.1589	0.085
H(3SA)	1.0428	0.9180	-0.0624	0.043
H(3SB)	0.9951	0.8590	-0.0818	0.043
H(4SA)	0.7237	0.8440	0.2711	0.054
H(4SB)	0.7717	0.9114	0.2540	0.054

Table 3. Anisotropic displacement parameters ($Å^2$) for 5a.
The anisotropic displacement factor exponent takes the form:
$-2\pi^2[h^2a^{*2}U_{11} + ... + 2hka^*b^*U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O(1A)	0.0351(10)	0.0714(14)	0.0242(9)	0.0073(9)	0.0004(8)	0.0116(9)
O(2A)	0.0242(10)	0.1021(19)	0.0334(11)	-0.0055(12)	0.0033(8)	-0.0153(11)
N(1A)	0.0214(10)	0.0230(9)	0.0325(11)	0.0053(8)	-0.0030(8)	0.0013(7)
N(2A)	0.0243(10)	0.0284(10)	0.0272(11)	0.0045(8)	0.0019(8)	0.0031(8)
C(1A)	0.0243(12)	0.0270(11)	0.0313(12)	0.0056(9)	0.0020(10)	0.0023(9)
C(2A)	0.0203(11)	0.0254(10)	0.0264(12)	0.0018(9)	-0.0017(9)	-0.0027(9)
C(3A)	0.0227(11)	0.0268(11)	0.0247(11)	0.0001(9)	0.0001(9)	-0.0008(8)
C(4A)	0.0210(11)	0.0307(12)	0.0279(12)	0.0046(10)	-0.0016(9)	0.0008(9)
C(5A)	0.0319(13)	0.0294(13)	0.0477(16)	0.0018(11)	-0.0104(12)	-0.0022(10)
C(6A)	0.0310(13)	0.0405(14)	0.0403(15)	-0.0011(12)	-0.0103(11)	-0.0054(11)
C(7A)	0.0261(12)	0.0487(15)	0.0304(13)	0.0050(11)	-0.0030(10)	0.0045(10)
C(8A)	0.0298(13)	0.0362(13)	0.0315(13)	0.0080(10)	0.0020(11)	0.0052(10)
C(9A)	0.0230(11)	0.0312(12)	0.0295(12)	0.0052(10)	0.0018(9)	0.0018(9)
C(10A)	0.064(2)	0.0284(14)	0.069(2)	0.0007(14)	-0.0310(18)	-0.0041(14)
C(11A)	0.076(3)	0.0364(17)	0.095(3)	-0.0145(18)	-0.032(2)	0.0064(16)
C(12A)	0.100(3)	0.0442(19)	0.074(3)	0.0185(19)	-0.015(2)	-0.022(2)
C(13A)	0.0378(14)	0.0278(12)	0.0376(14)	0.0016(11)	-0.0057(12)	0.0026(10)
C(14A)	0.072(2)	0.0467(18)	0.058(2)	-0.0101(16)	0.0114(18)	-0.0264(17)
C(15A)	0.057(2)	0.056(2)	0.059(2)	-0.0236(17)	-0.0007(17)	0.0124(16)
C(16A)	0.0320(13)	0.0395(14)	0.0237(12)	0.0085(10)	0.0064(10)	0.0055(10)
C(17A)	0.066(2)	0.0438(16)	0.0315(15)	0.0077(12)	0.0142(14)	0.0171(15)
C(18A)	0.089(3)	0.0501(19)	0.0344(17)	0.0005(14)	0.0179(17)	0.0211(18)
C(19A)	0.069(2)	0.068(2)	0.0298(15)	0.0136(15)	0.0118(15)	0.0157(18)
C(20A)	0.0469(17)	0.0501(18)	0.0352(15)	0.0144(13)	0.0080(13)	0.0092(13)
C(21A)	0.0284(12)	0.0371(13)	0.0341(13)	0.0076(11)	0.0025(10)	0.0026(10)
C(22A)	0.102(3)	0.0426(18)	0.0384(17)	0.0082(14)	0.0259(19)	0.0263(19)
C(23A)	0.045(2)	0.069(3)	0.306(12)	0.080(5)	0.009(4)	0.008(2)
C(24A)	0.057(2)	0.058(2)	0.128(4)	0.028(3)	-0.023(3)	0.0029(18)
C(25A)	0.0439(16)	0.0303(13)	0.0378(14)	0.0097(11)	0.0077(12)	0.0029(11)
C(26A)	0.0460(17)	0.0400(16)	0.0562(19)	0.0096(14)	0.0025(15)	0.0085(13)
C(27A)	0.067(2)	0.0450(18)	0.066(2)	-0.0038(16)	-0.0161(19)	0.0021(16)
C(28A)	0.0290(13)	0.0364(13)	0.0277(13)	0.0011(10)	0.0015(10)	-0.0052(10)
O(1B)	0.0382(12)	0.1010(19)	0.0272(10)	0.0133(12)	-0.0049(9)	0.0189(12)
O(2B)	0.0228(9)	0.0767(15)	0.0422(12)	0.0260(11)	0.0027(8)	0.0136(9)
N(1B)	0.0222(10)	0.0270(9)	0.0232(10)	0.0035(8)	-0.0011(8)	-0.0003(7)
N(2B)	0.0216(10)	0.0269(9)	0.0244(10)	0.0057(8)	-0.0017(8)	0.0000(7)
C(1B)	0.0220(11)	0.0254(11)	0.0260(11)	0.0008(9)	-0.0013(9)	0.0022(8)
C(2B)	0.0231(12)	0.0309(12)	0.0288(12)	0.0101(10)	-0.0007(10)	0.0024(9)
C(3B)	0.0194(11)	0.0342(12)	0.0318(13)	0.0136(10)	0.0001(9)	0.0027(9)
C(4B)	0.0231(12)	0.0395(13)	0.0222(12)	-0.0036(10)	-0.0036(9)	0.0076(10)
C(5B)	0.0264(13)	0.0571(17)	0.0245(13)	0.0064(11)	0.0019(10)	-0.0017(11)
C(6B)	0.0320(15)	0.107(3)	0.0268(14)	0.0090(17)	0.0055(12)	0.0028(16)
C(7B)	0.0439(19)	0.128(4)	0.0256(15)	-0.012(2)	0.0006(14)	0.037(2)

C(8B)	0.070(2)	0.083(3)	0.0354(17)	-0.0216(18)	-0.0137(17)	0.042(2)
C(9B)	0.0511(18)	0.0476(17)	0.0390(16)	-0.0141(13)	-0.0174(14)	0.0183(14)
C(10B)	0.0557(19)	0.0478(17)	0.0382(16)	0.0053(13)	0.0092(14)	-0.0189(14)
C(11B)	0.144(5)	0.047(2)	0.070(3)	0.010(2)	-0.021(3)	-0.012(3)
C(12B)	0.089(3)	0.110(4)	0.053(2)	-0.005(2)	-0.004(2)	-0.049(3)
C(13B)	0.086(3)	0.0390(17)	0.068(2)	-0.0175(17)	-0.028(2)	0.0058(17)
C(14B)	0.190(7)	0.084(4)	0.116(5)	0.004(4)	-0.083(5)	-0.052(4)
C(15B)	0.110(4)	0.060(2)	0.059(2)	-0.0034(19)	-0.007(2)	0.030(2)
C(16B)	0.0223(11)	0.0339(12)	0.0211(11)	0.0045(9)	-0.0019(9)	0.0009(9)
C(17B)	0.0219(11)	0.0365(13)	0.0292(13)	0.0107(10)	-0.0035(10)	-0.0016(9)
C(18B)	0.0290(13)	0.0522(16)	0.0310(14)	0.0153(12)	-0.0008(10)	-0.0063(11)
C(19B)	0.0308(13)	0.0605(18)	0.0248(13)	0.0044(12)	-0.0027(10)	-0.0041(12)
C(20B)	0.0393(15)	0.0495(16)	0.0294(13)	-0.0051(12)	-0.0060(11)	-0.0044(12)
C(21B)	0.0290(12)	0.0367(13)	0.0300(13)	0.0009(11)	-0.0003(10)	-0.0005(10)
C(22B)	0.0431(15)	0.0303(13)	0.0359(14)	0.0109(11)	-0.0065(12)	-0.0052(11)
C(23B)	0.0430(17)	0.0372(15)	0.068(2)	0.0161(15)	-0.0054(15)	-0.0091(12)
C(24B)	0.060(2)	0.0345(14)	0.0517(18)	0.0078(13)	0.0093(15)	-0.0013(13)
C(25B)	0.064(2)	0.0307(13)	0.0381(15)	-0.0008(12)	-0.0018(14)	-0.0118(13)
C(26B)	0.096(3)	0.0343(16)	0.077(3)	-0.0027(17)	0.007(2)	-0.0014(18)
C(27B)	0.062(2)	0.053(2)	0.069(2)	-0.0009(17)	0.0158(19)	-0.0226(17)
C(28B)	0.0248(13)	0.0627(18)	0.0268(13)	0.0195(12)	0.0009(10)	0.0036(12)
O(1C)	0.0349(10)	0.0674(14)	0.0283(10)	0.0018(9)	0.0055(8)	-0.0077(9)
O(2C)	0.0231(10)	0.119(2)	0.0435(12)	-0.0107(14)	-0.0003(9)	0.0176(12)
N(1C)	0.0221(10)	0.0297(10)	0.0309(11)	0.0069(8)	0.0055(8)	0.0004(8)
N(2C)	0.0258(10)	0.0282(10)	0.0292(11)	0.0057(8)	-0.0007(8)	-0.0003(8)
C(1C)	0.0214(12)	0.0306(12)	0.0361(14)	0.0098(10)	0.0001(10)	-0.0034(9)
C(2C)	0.0196(11)	0.0284(11)	0.0319(13)	0.0033(9)	0.0034(9)	0.0030(9)
C(3C)	0.0217(11)	0.0311(11)	0.0272(12)	0.0021(9)	0.0033(9)	0.0021(9)
C(4C)	0.0223(11)	0.0339(13)	0.0300(12)	0.0060(10)	0.0037(10)	-0.0010(9)
C(5C)	0.0280(13)	0.0396(15)	0.0494(17)	0.0036(12)	0.0144(12)	0.0025(11)
C(6C)	0.0324(14)	0.0505(17)	0.0408(16)	-0.0049(13)	0.0112(12)	0.0023(12)
C(7C)	0.0241(12)	0.0582(18)	0.0267(13)	0.0049(12)	-0.0012(10)	-0.0069(11)
C(8C)	0.0282(12)	0.0447(15)	0.0245(12)	0.0091(11)	-0.0041(10)	-0.0097(10)
C(9C)	0.0242(11)	0.0347(13)	0.0266(12)	0.0062(10)	-0.0027(10)	-0.0032(9)
C(10C)	0.068(2)	0.0349(16)	0.089(3)	-0.0016(17)	0.045(2)	0.0034(15)
C(11C)	0.147(5)	0.047(2)	0.071(3)	0.020(2)	0.038(3)	0.041(3)
C(12C)	0.065(2)	0.0390(18)	0.127(4)	-0.020(2)	0.023(3)	0.0013(17)
C(13C)	0.0464(16)	0.0283(13)	0.0401(15)	0.0031(11)	0.0098(13)	-0.0011(11)
C(14C)	0.079(3)	0.054(2)	0.063(2)	-0.0179(18)	0.019(2)	-0.0223(19)
C(15C)	0.087(3)	0.065(2)	0.070(3)	0.013(2)	0.007(2)	0.042(2)
C(16C)	0.0287(12)	0.0331(13)	0.0288(13)	0.0047(10)	-0.0041(10)	-0.0021(10)
C(17C)	0.0497(17)	0.0392(15)	0.0356(15)	0.0060(12)	-0.0107(13)	-0.0096(12)
C(18C)	0.071(2)	0.055(2)	0.0369(17)	0.0038(14)	-0.0185(16)	-0.0173(17)
C(19C)	0.063(2)	0.0566(19)	0.0320(15)	0.0084(14)	-0.0113(14)	-0.0111(16)
C(20C)	0.0428(16)	0.0436(16)	0.0365(15)	0.0140(12)	-0.0049(12)	-0.0065(12)
C(21C)	0.0281(12)	0.0335(13)	0.0364(14)	0.0084(11)	-0.0027(10)	-0.0030(10)
C(22C)	0.079(2)	0.0369(15)	0.0390(16)	0.0059(13)	-0.0166(16)	-0.0188(15)
C(23C)	0.052(2)	0.055(2)	0.104(3)	0.022(2)	0.019(2)	-0.0094(17)
C(24C)	0.047(2)	0.058(2)	0.130(4)	0.021(3)	-0.004(2)	-0.0037(17)

C(25C)	0.0439(16)	0.0311(13)	0.0372(14)	0.0071(11)	-0.0001(12)	-0.0029(11)
C(26C)	0.067(2)	0.0445(18)	0.072(3)	-0.0051(17)	0.026(2)	-0.0024(16)
C(27C)	0.0485(17)	0.0348(15)	0.0544(19)	0.0063(13)	-0.0051(14)	-0.0058(12)
C(28C)	0.0277(12)	0.0402(13)	0.0277(13)	0.0046(10)	0.0003(10)	0.0017(10)
O(1D)	0.0402(12)	0.109(2)	0.0254(10)	-0.0151(12)	0.0040(9)	0.0159(13)
O(2D)	0.0251(10)	0.0773(16)	0.0437(12)	-0.0247(11)	-0.0011(9)	0.0125(10)
N(1D)	0.0219(10)	0.0278(10)	0.0215(9)	-0.0019(8)	0.0031(8)	-0.0020(7)
N(2D)	0.0229(10)	0.0250(9)	0.0244(10)	-0.0032(8)	0.0027(8)	-0.0009(7)
C(1D)	0.0220(11)	0.0243(10)	0.0261(11)	0.0011(9)	0.0042(9)	-0.0005(8)
C(2D)	0.0226(12)	0.0329(12)	0.0302(12)	-0.0121(10)	0.0001(10)	0.0012(9)
C(3D)	0.0248(12)	0.0345(12)	0.0266(12)	-0.0111(10)	-0.0002(9)	0.0017(9)
C(4D)	0.0238(12)	0.0408(13)	0.0211(11)	0.0030(10)	0.0035(9)	0.0078(10)
C(5D)	0.0550(19)	0.0520(18)	0.0365(16)	0.0151(14)	0.0177(14)	0.0176(15)
C(6D)	0.071(2)	0.089(3)	0.0327(17)	0.0240(19)	0.0139(17)	0.044(2)
C(7D)	0.055(2)	0.137(4)	0.0234(15)	0.018(2)	0.0031(15)	0.051(3)
C(8D)	0.0347(16)	0.103(3)	0.0308(15)	-0.0067(18)	-0.0057(13)	-0.0013(16)
C(9D)	0.0255(13)	0.0559(17)	0.0271(13)	0.0007(12)	-0.0041(11)	0.0004(11)
C(10D)	0.085(3)	0.0378(17)	0.070(2)	0.0209(17)	0.023(2)	0.0055(17)
C(11D)	0.122(4)	0.062(2)	0.058(2)	0.007(2)	-0.001(3)	0.034(3)
C(12D)	0.233(9)	0.069(3)	0.162(7)	0.004(4)	0.123(7)	-0.050(5)
C(13D)	0.059(2)	0.0480(17)	0.0403(17)	-0.0061(14)	-0.0060(15)	-0.0214(15)
C(14D)	0.092(3)	0.117(4)	0.052(2)	0.015(3)	0.002(2)	-0.057(3)
C(15D)	0.162(6)	0.045(2)	0.071(3)	-0.013(2)	0.016(3)	-0.018(3)
C(16D)	0.0239(11)	0.0304(11)	0.0213(11)	-0.0021(9)	0.0008(9)	0.0013(9)
C(17D)	0.0334(13)	0.0295(12)	0.0340(14)	0.0011(11)	0.0036(11)	-0.0006(10)
C(18D)	0.0345(14)	0.0401(14)	0.0330(14)	0.0102(11)	0.0022(11)	0.0038(11)
C(19D)	0.0402(15)	0.0556(17)	0.0222(12)	-0.0032(12)	0.0030(11)	0.0047(12)
C(20D)	0.0405(15)	0.0411(14)	0.0287(13)	-0.0099(11)	-0.0001(11)	-0.0017(11)
C(21D)	0.0269(12)	0.0293(12)	0.0285(12)	-0.0050(10)	0.0050(10)	-0.0002(9)
C(22D)	0.063(2)	0.0353(15)	0.0430(17)	0.0016(13)	0.0105(15)	-0.0126(14)
C(23D)	0.077(3)	0.065(2)	0.084(3)	0.012(2)	-0.025(2)	-0.038(2)
C(24D)	0.098(3)	0.0309(17)	0.097(3)	0.0045(18)	0.003(3)	-0.0011(18)
C(25D)	0.0548(17)	0.0301(13)	0.0319(13)	-0.0054(11)	0.0116(12)	-0.0088(12)
C(26D)	0.064(2)	0.0308(14)	0.0530(19)	0.0052(13)	-0.0099(16)	-0.0043(13)
C(27D)	0.0493(18)	0.0353(15)	0.065(2)	-0.0127(14)	0.0148(16)	-0.0105(13)
C(28D)	0.0240(13)	0.0584(17)	0.0330(14)	-0.0193(13)	0.0009(11)	0.0029(11)
O(1S)	0.0476(12)	0.0665(15)	0.0399(12)	0.0086(10)	-0.0005(10)	0.0033(11)
O(2S)	0.0647(17)	0.103(2)	0.0471(15)	-0.0120(14)	0.0174(13)	-0.0179(15)
C(1S)	0.060(2)	0.054(2)	0.089(3)	0.021(2)	0.007(2)	0.0146(18)
Cl(1S)	0.0945(8)	0.0626(6)	0.0675(7)	0.0183(5)	-0.0003(6)	-0.0098(5)
Cl(2S)	0.1296(12)	0.0547(6)	0.0884(9)	0.0146(6)	0.0545(8)	0.0201(6)
C(2S)	0.067(3)	0.058(2)	0.088(3)	-0.026(2)	-0.009(2)	-0.0068(19)
Cl(3S)	0.1154(11)	0.0581(6)	0.1072(11)	0.0207(6)	-0.0489(8)	-0.0243(6)
Cl(4S)	0.217(2)	0.0854(10)	0.1195(14)	-0.0562(10)	-0.0664(14)	0.0671(12)
Cl(5S)	0.054(2)	0.0386(18)	0.069(3)	-0.0161(17)	-0.0319(19)	0.0125(15)
Cl(6S)	0.0430(19)	0.0367(17)	0.048(2)	0.0114(14)	-0.0001(14)	-0.0039(13)

Table 4. Bond lengths [Å] for 5a.

atom-atom	distance	atom-atom	distance	
O(1A)-C(28A)	1.227(3)	O(2A)-C(28A)	1.243(3)	N(1A)-
C(1A)	1.326(3)	N(1A)-C(2A)	1.399(3)	N(1A)-
C(4A)	1.453(3)	N(2A)-C(1A)	1.339(3)	N(2A)-
C(3A)	1.384(3)	N(2A)-C(16A)	1.456(3)	C(2A)-
C(3A)	1.347(3)	C(2A)-C(28A)	1.513(3)	C(4A)-
C(5A)	1.387(4)	C(4A)-C(9A)	1.391(3)	C(5A)-
C(6A)	1.407(4)	C(5A)-C(10A)	1.509(4)	C(6A)-
C(7A)	1.381(4)	C(7A)-C(8A)	1.383(4)	C(8A)-
C(9A)	1.393(4)	C(9A)-C(13A)	1.524(4)	C(10A)-
C(11A)	1.520(6)	C(10A)-C(12A)	1.543(6)	C(13A)-
C(14A)	1.512(4)	C(13A)-C(15A)	1.529(4)	C(16A)-
C(17A)	1.381(4)	C(16A)-C(21A)	1.407(4)	C(17A)-
C(18A)	1.400(5)	C(17A)-C(22A)	1.525(4)	C(18A)-
C(19A)	1.380(5)	C(19A)-C(20A)	1.374(5)	C(20A)-
C(21A)	1.392(4)	C(21A)-C(25A)	1.521(4)	C(22A)-
C(24A)	1.481(6)	C(22A)-C(23A)	1.511(8)	C(25A)-
C(27A)	1.520(5)	C(25A)-C(26A)	1.536(4)	O(1B)-
C(28B)	1.238(4)	O(2B)-C(28B)	1.250(4)	N(1B)-
C(1B)	1.331(3)	N(1B)-C(2B)	1.384(3)	N(1B)-
C(4B)	1.456(3)	N(2B)-C(1B)	1.336(3)	N(2B)-
C(3B)	1.382(3)	N(2B)-C(16B)	1.451(3)	C(2B)-
C(3B)	1.353(4)	C(2B)-C(28B)	1.516(3)	C(4B)-
C(5B)	1.394(4)	C(4B)-C(9B)	1.395(4)	C(5B)-
C(6B)	1.411(4)	C(5B)-C(10B)	1.513(5)	C(6B)-
C(7B)	1.372(6)	C(7B)-C(8B)	1.379(7)	C(8B)-
C(9B)	1.383(5)	C(9B)-C(13B)	1.504(6)	C(10B)-
C(12B)	1.529(5)	C(10B)-C(11B)	1.539(6)	C(13B)-
C(15B)	1.526(6)	C(13B)-C(14B)	1.531(6)	C(16B)-
C(21B)	1.390(4)	C(16B)-C(17B)	1.403(3)	C(17B)-
C(18B)	1.394(4)	C(17B)-C(22B)	1.520(4)	C(18B)-
C(19B)	1.372(4)	C(19B)-C(20B)	1.385(4)	C(20B)-
C(21B)	1.389(4)	C(21B)-C(25B)	1.513(4)	C(22B)-
C(23B)	1.535(4)	C(22B)-C(24B)	1.536(5)	C(25B)-
C(27B)	1.531(5)	C(25B)-C(26B)	1.539(5)	O(1C)-
C(28C)	1.242(3)	O(2C)-C(28C)	1.224(3)	N(1C)-
C(1C)	1.331(3)	N(1C)-C(2C)	1.401(3)	N(1C)-
C(4C)	1.455(3)	N(2C)-C(1C)	1.339(3)	N(2C)-
C(3C)	1.379(3)	N(2C)-C(16C)	1.450(3)	C(2C)-
C(3C)	1.361(4)	C(2C)-C(28C)	1.507(4)	C(4C)-
C(9C)	1.393(4)	C(4C)-C(5C)	1.401(4)	C(5C)-
C(6C)	1.394(4)	C(5C)-C(10C)	1.511(4)	C(6C)-
C(7C)	1.373(4)	C(7C)-C(8C)	1.376(4)	C(8C)-
C(9C)	1.400(4)	C(9C)-C(13C)	1.518(4)	C(10C)-
C(11C)	1.542(8)	C(10C)-C(12C)	1.551(6)	C(13C)-
C(15C)	1.519(5)	C(13C)-C(14C)	1.527(5)	C(16C)-

C(21C)	1.407(4)	C(16C)-C(17C)	1.407(4)	C(17C)-
C(18C)	1.393(4)	C(17C)-C(22C)	1.515(4)	C(18C)-
C(19C)	1.384(5)	C(19C)-C(20C)	1.379(5)	C(20C)-
C(21C)	1.390(4)	C(21C)-C(25C)	1.514(4)	C(22C)-
C(23C)	1.514(5)	C(22C)-C(24C)	1.563(6)	C(25C)-
C(27C)	1.534(4)	C(25C)-C(26C)	1.534(5)	O(1D)-
C(28D)	1.242(4)	O(2D)-C(28D)	1.256(4)	N(1D)-
C(1D)	1.335(3)	N(1D)-C(2D)	1.393(3)	N(1D)-
C(4D)	1.452(3)	N(2D)-C(1D)	1.323(3)	N(2D)-
C(3D)	1.379(3)	N(2D)-C(16D)	1.456(3)	C(2D)-
C(3D)	1.356(4)	C(2D)-C(28D)	1.511(4)	C(4D)-
C(9D)	1.389(4)	C(4D)-C(5D)	1.392(4)	C(5D)-
C(6D)	1.379(5)	C(5D)-C(10D)	1.519(6)	C(6D)-
C(7D)	1.381(7)	C(7D)-C(8D)	1.377(7)	C(8D)-
C(9D)	1.395(4)	C(9D)-C(13D)	1.505(5)	C(10D)-
C(12D)	1.519(6)	C(10D)-C(11D)	1.532(6)	C(13D)-
C(15D)	1.511(6)	C(13D)-C(14D)	1.539(5)	C(16D)-
C(17D)	1.395(4)	C(16D)-C(21D)	1.397(3)	C(17D)-
C(18D)	1.399(4)	C(17D)-C(22D)	1.508(4)	C(18D)-
C(19D)	1.384(4)	C(19D)-C(20D)	1.369(4)	C(20D)-
C(21D)	1.396(4)	C(21D)-C(25D)	1.520(4)	C(22D)-
C(24D)	1.535(5)	C(22D)-C(23D)	1.543(6)	C(25D)-
C(26D)	1.528(5)	C(25D)-C(27D)	1.533(4)	C(1S)-
Cl(2S)	1.739(5)	C(1S)-Cl(1S)	1.775(5)	C(2S)-
Cl(4S)	1.724(4)	C(2S)-Cl(3S)	1.777(6)	C(3S)-
Cl(6S)	1.774(15)	C(3S)-Cl(5S)	1.784(14)	C(4S)-
Cl(7S)	1.719(18)	C(4S)-Cl(8S)	1.785(17)	C(1A)-
H(1A)	0.9500	C(3A)-H(3A)	0.9500	C(6A)-
H(6A)	0.9500	C(7A)-H(7A)	0.9500	C(8A)-
H(8A)	0.9500	C(10A)-H(10A)	1.0000	C(11A)-
H(11A)	0.9800	C(11A)-H(11B)	0.9800	C(11A)-
H(11C)	0.9800	C(12A)-H(12A)	0.9800	C(12A)-
H(12B)	0.9800	C(12A)-H(12C)	0.9800	C(13A)-
H(13A)	1.0000	C(14A)-H(14A)	0.9800	C(14A)-
H(14B)	0.9800	C(14A)-H(14C)	0.9800	C(15A)-
H(15A)	0.9800	C(15A)-H(15B)	0.9800	C(15A)-
H(15C)	0.9800	C(18A)-H(18A)	0.9500	C(19A)-
H(19A)	0.9500	C(20A)-H(20A)	0.9500	C(22A)-
H(22A)	1.0000	C(23A)-H(23A)	0.9800	C(23A)-
H(23B)	0.9800	C(23A)-H(23C)	0.9800	C(24A)-
H(24A)	0.9800	C(24A)-H(24B)	0.9800	C(24A)-
H(24C)	0.9800	C(25A)-H(25A)	1.0000	C(26A)-
H(26A)	0.9800	C(26A)-H(26B)	0.9800	C(26A)-
H(26C)	0.9800	C(27A)-H(27A)	0.9800	C(27A)-
H(27B)	0.9800	C(27A)-H(27C)	0.9800	C(1B)-
H(1B)	0.9500	C(3B)-H(3B)	0.9500	C(6B)-
H(6B)	0.9500	C(7B)-H(7B)	0.9500	C(8B)-
H(8B)	0.9500	C(10B)-H(10B)	1.0000	C(11B)-
H(11D)	0.9800	C(11B)-H(11E)	0.9800	C(11B)-

H(11F)	0.9800	C(12B)-H(12D)	0.9800	C(12B)-
H(12E)	0.9800	C(12B)-H(12F)	0.9800	C(13B)-
H(13B)	1.0000	C(14B)-H(14D)	0.9800	C(14B)-
H(14E)	0.9800	C(14B)-H(14F)	0.9800	C(15B)-
H(15D)	0.9800	C(15B)-H(15E)	0.9800	C(15B)-
H(15F)	0.9800	C(18B)-H(18B)	0.9500	C(19B)-
H(19B)	0.9500	C(20B)-H(20B)	0.9500	C(22B)-
H(22B)	1.0000	C(23B)-H(23D)	0.9800	C(23B)-
H(23E)	0.9800	C(23B)-H(23F)	0.9800	C(24B)-
H(24D)	0.9800	C(24B)-H(24E)	0.9800	C(24B)-
H(24F)	0.9800	C(25B)-H(25B)	1.0000	C(26B)-
H(26D)	0.9800	C(26B)-H(26E)	0.9800	C(26B)-
H(26F)	0.9800	C(27B)-H(27D)	0.9800	C(27B)-
H(27E)	0.9800	C(27B)-H(27F)	0.9800	C(1C)-
H(1C)	0.9500	C(3C)-H(3C)	0.9500	C(6C)-
H(6C)	0.9500	C(7C)-H(7C)	0.9500	C(8C)-
H(8C)	0.9500	C(10C)-H(10C)	1.0000	C(11C)-
H(11G)	0.9814	C(11C)-H(11H)	0.9794	C(11C)-
H(11I)	0.9814	C(11C)-H(11X)	0.9801	C(11C)-
H(11Y)	0.9821	C(11C)-H(11Z)	0.9800	C(12C)-
H(12G)	0.9800	C(12C)-H(12H)	0.9800	C(12C)-
H(12I)	0.9800	C(13C)-H(13C)	1.0000	C(14C)-
H(14G)	0.9800	C(14C)-H(14H)	0.9800	C(14C)-
H(14I)	0.9800	C(15C)-H(15G)	0.9800	C(15C)-
H(15H)	0.9800	C(15C)-H(15I)	0.9800	C(18C)-
H(18C)	0.9500	C(19C)-H(19C)	0.9500	C(20C)-
H(20C)	0.9500	C(22C)-H(22C)	1.0000	C(23C)-
H(23G)	0.9800	C(23C)-H(23H)	0.9800	C(23C)-
H(23I)	0.9800	C(24C)-H(24G)	0.9800	C(24C)-
H(24H)	0.9800	C(24C)-H(24I)	0.9800	C(25C)-
H(25C)	1.0000	C(26C)-H(26G)	0.9800	C(26C)-
H(26H)	0.9800	C(26C)-H(26I)	0.9800	C(27C)-
H(27G)	0.9800	C(27C)-H(27H)	0.9800	C(27C)-
H(27I)	0.9800	C(1D)-H(1D)	0.9500	C(3D)-
H(3D)	0.9500	C(6D)-H(6D)	0.9500	C(7D)-
H(7D)	0.9500	C(8D)-H(8D)	0.9500	C(10D)-
H(10D)	1.0000	C(11D)-H(11J)	0.9800	C(11D)-
H(11K)	0.9800	C(11D)-H(11L)	0.9800	C(12D)-
H(12J)	0.9800	C(12D)-H(12K)	0.9800	C(12D)-
H(12L)	0.9800	C(13D)-H(13D)	1.0000	C(14D)-
H(14J)	0.9800	C(14D)-H(14K)	0.9800	C(14D)-
H(14L)	0.9800	C(15D)-H(15J)	0.9800	C(15D)-
H(15K)	0.9800	C(15D)-H(15L)	0.9800	C(18D)-
H(18D)	0.9500	C(19D)-H(19D)	0.9500	C(20D)-
H(20D)	0.9500	C(22D)-H(22D)	1.0000	C(23D)-
H(23J)	0.9800	C(23D)-H(23K)	0.9800	C(23D)-
H(23L)	0.9800	C(24D)-H(24J)	0.9800	C(24D)-
H(24K)	0.9800	C(24D)-H(24L)	0.9800	C(25D)-
H(25D)	1.0000	C(26D)-H(26J)	0.9800	C(26D)-

H(26K)	0.9800	C(26D)-H(26L)	0.9800	C(27D)-
H(27J)	0.9800	C(27D)-H(27K)	0.9800	C(27D)-
H(27L)	0.9800	C(1S)-H(1SA)	0.9900	C(1S)-
H(1SB)	0.9900	C(2S)-H(2SA)	0.9900	C(2S)-
H(2SB)	0.9900	C(3S)-H(3SA)	0.9900	C(3S)-
H(3SB)	0.9900	C(4S)-H(4SA)	0.9900	C(4S)-
H(4SB)	0.9900			

Table 5. Bond angles [°] for 5a.

atom-atom-atom	angle	atom-atom-atom	angle	
C(1A)-N(1A)-C(2A)	109.0(2)	C(1A)-N(1A)-C(4A)	123.8(2)	C(2A)-
N(1A)-C(4A)	126.6(2)	C(1A)-N(2A)-C(3A)	108.5(2)	C(1A)-
N(2A)-C(16A)	125.1(2)	C(3A)-N(2A)-C(16A)	126.4(2)	N(1A)-
C(1A)-N(2A)	108.4(2)	C(3A)-C(2A)-N(1A)	106.4(2)	C(3A)-
C(2A)-C(28A)	128.1(2)	N(1A)-C(2A)-C(28A)	125.4(2)	C(2A)-
C(3A)-N(2A)	107.6(2)	C(5A)-C(4A)-C(9A)	123.9(2)	C(5A)-
C(4A)-N(1A)	118.5(2)	C(9A)-C(4A)-N(1A)	117.5(2)	C(4A)-
C(5A)-C(6A)	116.7(2)	C(4A)-C(5A)-C(10A)	122.4(3)	C(6A)-
C(5A)-C(10A)	120.9(3)	C(7A)-C(6A)-C(5A)	121.1(3)	C(6A)-
C(7A)-C(8A)	119.9(3)	C(7A)-C(8A)-C(9A)	121.4(2)	C(4A)-
C(9A)-C(8A)	116.9(2)	C(4A)-C(9A)-C(13A)	122.6(2)	C(8A)-
C(9A)-C(13A)	120.5(2)	C(5A)-C(10A)-C(11A)	112.7(3)	C(5A)-
C(10A)-C(12A)	110.6(3)	C(11A)-C(10A)-C(12A)	110.6(3)	C(14A)-
C(13A)-C(9A)	112.3(2)	C(14A)-C(13A)-C(15A)	111.7(3)	C(9A)-
C(13A)-C(15A)	110.7(2)	C(17A)-C(16A)-C(21A)	123.8(3)	C(17A)-
C(16A)-N(2A)	118.8(2)	C(21A)-C(16A)-N(2A)	117.5(2)	C(16A)-
C(17A)-C(18A)	116.3(3)	C(16A)-C(17A)-C(22A)	123.6(3)	C(18A)-
C(17A)-C(22A)	120.0(3)	C(19A)-C(18A)-C(17A)	121.6(3)	C(20A)-
C(19A)-C(18A)	120.4(3)	C(19A)-C(20A)-C(21A)	120.9(3)	C(20A)-
C(21A)-C(16A)	117.0(3)	C(20A)-C(21A)-C(25A)	121.1(3)	C(16A)-
C(21A)-C(25A)	121.9(2)	C(24A)-C(22A)-C(23A)	108.3(4)	C(24A)-
C(22A)-C(17A)	112.0(3)	C(23A)-C(22A)-C(17A)	112.2(4)	C(27A)-
C(25A)-C(21A)	111.0(3)	C(27A)-C(25A)-C(26A)	109.8(3)	C(21A)-
C(25A)-C(26A)	113.1(3)	O(1A)-C(28A)-O(2A)	128.2(3)	O(1A)-
C(28A)-C(2A)	117.8(2)	O(2A)-C(28A)-C(2A)	113.9(2)	C(1B)-
N(1B)-C(2B)	109.5(2)	C(1B)-N(1B)-C(4B)	122.6(2)	C(2B)-
N(1B)-C(4B)	127.8(2)	C(1B)-N(2B)-C(3B)	108.6(2)	C(1B)-
N(2B)-C(16B)	126.4(2)	C(3B)-N(2B)-C(16B)	125.0(2)	N(1B)-
C(1B)-N(2B)	108.1(2)	C(3B)-C(2B)-N(1B)	106.3(2)	C(3B)-
C(2B)-C(28B)	129.2(2)	N(1B)-C(2B)-C(28B)	124.5(2)	C(2B)-
C(3B)-N(2B)	107.6(2)	C(5B)-C(4B)-C(9B)	124.1(3)	C(5B)-
C(4B)-N(1B)	117.5(2)	C(9B)-C(4B)-N(1B)	118.4(3)	C(4B)-
C(5B)-C(6B)	115.8(3)	C(4B)-C(5B)-C(10B)	123.0(2)	C(6B)-
C(5B)-C(10B)	121.3(3)	C(7B)-C(6B)-C(5B)	121.2(4)	C(6B)-
C(7B)-C(8B)	120.8(3)	C(7B)-C(8B)-C(9B)	120.9(4)	C(8B)-
C(9B)-C(4B)	117.2(4)	C(8B)-C(9B)-C(13B)	120.5(3)	C(4B)-
C(9B)-C(13B)	122.3(3)	C(5B)-C(10B)-C(12B)	110.7(4)	C(5B)-
C(10B)-C(11B)	110.1(3)	C(12B)-C(10B)-C(11B)	111.5(3)	C(9B)-
C(13B)-C(15B)	109.8(4)	C(9B)-C(13B)-C(14B)	112.0(4)	C(15B)-
C(13B)-C(14B)	112.2(4)	C(21B)-C(16B)-C(17B)	123.9(2)	C(21B)-
C(16B)-N(2B)	117.9(2)	C(17B)-C(16B)-N(2B)	118.1(2)	C(18B)-
C(17B)-C(16B)	116.3(3)	C(18B)-C(17B)-C(22B)	121.7(2)	C(16B)-
C(17B)-C(22B)	121.9(2)	C(19B)-C(18B)-C(17B)	121.0(3)	C(18B)-
C(19B)-C(20B)	121.2(3)	C(19B)-C(20B)-C(21B)	120.4(3)	C(20B)-
C(21B)-C(16B)	117.1(3)	C(20B)-C(21B)-C(25B)	120.9(3)	C(16B)-

C(21B)-C(25B)	121.9(2)	C(17B)-C(22B)-C(23B)	113.8(3)	C(17B)-
C(22B)-C(24B)	109.8(2)	C(23B)-C(22B)-C(24B)	109.6(2)	C(21B)-
C(25B)-C(27B)	109.5(3)	C(21B)-C(25B)-C(26B)	113.2(3)	C(27B)-
C(25B)-C(26B)	111.3(3)	O(1B)-C(28B)-O(2B)	130.1(3)	O(1B)-
C(28B)-C(2B)	116.1(2)	O(2B)-C(28B)-C(2B)	113.8(3)	C(1C)-
N(1C)-C(2C)	109.4(2)	C(1C)-N(1C)-C(4C)	122.2(2)	C(2C)-
N(1C)-C(4C)	127.4(2)	C(1C)-N(2C)-C(3C)	108.5(2)	C(1C)-
N(2C)-C(16C)	124.7(2)	C(3C)-N(2C)-C(16C)	126.8(2)	N(1C)-
C(1C)-N(2C)	108.4(2)	C(3C)-C(2C)-N(1C)	105.4(2)	C(3C)-
C(2C)-C(28C)	128.2(2)	N(1C)-C(2C)-C(28C)	126.1(2)	C(2C)-
C(3C)-N(2C)	108.3(2)	C(9C)-C(4C)-C(5C)	123.4(2)	C(9C)-
C(4C)-N(1C)	117.4(2)	C(5C)-C(4C)-N(1C)	119.2(2)	C(6C)-
C(5C)-C(4C)	116.6(3)	C(6C)-C(5C)-C(10C)	122.5(3)	C(4C)-
C(5C)-C(10C)	120.9(3)	C(7C)-C(6C)-C(5C)	121.7(3)	C(6C)-
C(7C)-C(8C)	120.1(3)	C(7C)-C(8C)-C(9C)	121.4(3)	C(4C)-
C(9C)-C(8C)	116.8(2)	C(4C)-C(9C)-C(13C)	122.9(2)	C(8C)-
C(9C)-C(13C)	120.3(2)	C(5C)-C(10C)-C(11C)	110.3(4)	C(5C)-
C(10C)-C(12C)	111.0(4)	C(11C)-C(10C)-C(12C)	111.5(3)	C(9C)-
C(13C)-C(15C)	110.4(3)	C(9C)-C(13C)-C(14C)	111.5(3)	C(15C)-
C(13C)-C(14C)	112.5(3)	C(21C)-C(16C)-C(17C)	123.5(3)	C(21C)-
C(16C)-N(2C)	118.2(2)	C(17C)-C(16C)-N(2C)	118.3(2)	C(18C)-
C(17C)-C(16C)	116.7(3)	C(18C)-C(17C)-C(22C)	120.3(3)	C(16C)-
C(17C)-C(22C)	123.0(3)	C(19C)-C(18C)-C(17C)	121.1(3)	C(20C)-
C(19C)-C(18C)	120.6(3)	C(19C)-C(20C)-C(21C)	121.5(3)	C(20C)-
C(21C)-C(16C)	116.5(3)	C(20C)-C(21C)-C(25C)	121.6(2)	C(16C)-
C(21C)-C(25C)	121.8(2)	C(23C)-C(22C)-C(17C)	110.8(3)	C(23C)-
C(22C)-C(24C)	106.6(3)	C(17C)-C(22C)-C(24C)	111.6(3)	C(21C)-
C(25C)-C(27C)	112.9(3)	C(21C)-C(25C)-C(26C)	110.9(3)	C(27C)-
C(25C)-C(26C)	110.2(3)	O(2C)-C(28C)-O(1C)	128.2(3)	O(2C)-
C(28C)-C(2C)	114.6(2)	O(1C)-C(28C)-C(2C)	117.1(2)	C(1D)-
N(1D)-C(2D)	108.9(2)	C(1D)-N(1D)-C(4D)	123.3(2)	C(2D)-
N(1D)-C(4D)	127.7(2)	C(1D)-N(2D)-C(3D)	108.8(2)	C(1D)-
N(2D)-C(16D)	126.2(2)	C(3D)-N(2D)-C(16D)	125.0(2)	N(2D)-
C(1D)-N(1D)	108.7(2)	C(3D)-C(2D)-N(1D)	105.9(2)	C(3D)-
C(2D)-C(28D)	129.6(2)	N(1D)-C(2D)-C(28D)	124.5(2)	C(2D)-
C(3D)-N(2D)	107.8(2)	C(9D)-C(4D)-C(5D)	123.2(3)	C(9D)-
C(4D)-N(1D)	118.2(2)	C(5D)-C(4D)-N(1D)	118.7(3)	C(6D)-
C(5D)-C(4D)	117.7(4)	C(6D)-C(5D)-C(10D)	119.9(3)	C(4D)-
C(5D)-C(10D)	122.4(3)	C(5D)-C(6D)-C(7D)	121.0(4)	C(8D)-
C(7D)-C(6D)	119.9(3)	C(7D)-C(8D)-C(9D)	121.5(4)	C(4D)-
C(9D)-C(8D)	116.7(3)	C(4D)-C(9D)-C(13D)	122.6(2)	C(8D)-
C(9D)-C(13D)	120.7(3)	C(5D)-C(10D)-C(12D)	110.1(4)	C(5D)-
C(10D)-C(11D)	110.2(4)	C(12D)-C(10D)-C(11D)	112.7(4)	C(9D)-
C(13D)-C(15D)	111.1(3)	C(9D)-C(13D)-C(14D)	111.2(4)	C(15D)-
C(13D)-C(14D)	110.8(4)	C(17D)-C(16D)-C(21D)	124.2(2)	C(17D)-
C(16D)-N(2D)	117.8(2)	C(21D)-C(16D)-N(2D)	118.0(2)	C(16D)-
C(17D)-C(18D)	116.3(2)	C(16D)-C(17D)-C(22D)	122.4(2)	C(18D)-
C(17D)-C(22D)	121.2(3)	C(19D)-C(18D)-C(17D)	121.1(3)	C(20D)-
C(19D)-C(18D)	120.6(3)	C(19D)-C(20D)-C(21D)	121.5(3)	C(20D)-

C(21D)-C(16D)	116.3(2)	C(20D)-C(21D)-C(25D)	121.7(2)	C(16D)-
C(21D)-C(25D)	121.9(2)	C(17D)-C(22D)-C(24D)	112.8(3)	C(17D)-
C(22D)-C(23D)	108.9(3)	C(24D)-C(22D)-C(23D)	110.9(3)	C(21D)-
C(25D)-C(26D)	109.2(2)	C(21D)-C(25D)-C(27D)	113.4(3)	C(26D)-
C(25D)-C(27D)	109.4(2)	O(1D)-C(28D)-O(2D)	130.4(3)	O(1D)-
C(28D)-C(2D)	116.0(2)	O(2D)-C(28D)-C(2D)	113.6(3)	Cl(2S)-
C(1S)-Cl(1S)	112.2(2)	Cl(4S)-C(2S)-Cl(3S)	111.9(3)	Cl(6S)-
C(3S)-Cl(5S)	109.9(8)	Cl(7S)-C(4S)-Cl(8S)	112.5(10)	N(1A)-
C(1A)-H(1A)	125.8	N(2A)-C(1A)-H(1A)	125.8	C(2A)-
C(3A)-H(3A)	126.2	N(2A)-C(3A)-H(3A)	126.2	C(7A)-
C(6A)-H(6A)	119.4	C(5A)-C(6A)-H(6A)	119.4	C(6A)-
C(7A)-H(7A)	120.1	C(8A)-C(7A)-H(7A)	120.1	C(7A)-
C(8A)-H(8A)	119.3	C(9A)-C(8A)-H(8A)	119.3	C(5A)-
C(10A)-H(10A)	107.6	C(11A)-C(10A)-H(10A)	107.6	C(12A)-
C(10A)-H(10A)	107.6	C(10A)-C(11A)-H(11A)	109.5	C(10A)-
C(11A)-H(11B)	109.5	H(11A)-C(11A)-H(11B)	109.5	C(10A)-
C(11A)-H(11C)	109.5	H(11A)-C(11A)-H(11C)	109.5	H(11B)-
C(11A)-H(11C)	109.5	C(10A)-C(12A)-H(12A)	109.5	C(10A)-
C(12A)-H(12B)	109.5	H(12A)-C(12A)-H(12B)	109.5	C(10A)-
C(12A)-H(12C)	109.5	H(12A)-C(12A)-H(12C)	109.5	H(12B)-
C(12A)-H(12C)	109.5	C(14A)-C(13A)-H(13A)	107.3	C(9A)-
C(13A)-H(13A)	107.3	C(15A)-C(13A)-H(13A)	107.3	C(13A)-
C(14A)-H(14A)	109.5	C(13A)-C(14A)-H(14B)	109.5	H(14A)-
C(14A)-H(14B)	109.5	C(13A)-C(14A)-H(14C)	109.5	H(14A)-
C(14A)-H(14C)	109.5	H(14B)-C(14A)-H(14C)	109.5	C(13A)-
C(15A)-H(15A)	109.5	C(13A)-C(15A)-H(15B)	109.5	H(15A)-
C(15A)-H(15B)	109.5	C(13A)-C(15A)-H(15C)	109.5	H(15A)-
C(15A)-H(15C)	109.5	H(15B)-C(15A)-H(15C)	109.5	C(19A)-
C(18A)-H(18A)	119.2	C(17A)-C(18A)-H(18A)	119.2	C(20A)-
C(19A)-H(19A)	119.8	C(18A)-C(19A)-H(19A)	119.8	C(19A)-
C(20A)-H(20A)	119.6	C(21A)-C(20A)-H(20A)	119.6	C(24A)-
C(22A)-H(22A)	108.1	C(23A)-C(22A)-H(22A)	108.1	C(17A)-
C(22A)-H(22A)	108.1	C(22A)-C(23A)-H(23A)	109.5	C(22A)-
C(23A)-H(23B)	109.5	H(23A)-C(23A)-H(23B)	109.5	C(22A)-
C(23A)-H(23C)	109.5	H(23A)-C(23A)-H(23C)	109.5	H(23B)-
C(23A)-H(23C)	109.5	C(22A)-C(24A)-H(24A)	109.5	C(22A)-
C(24A)-H(24B)	109.5	H(24A)-C(24A)-H(24B)	109.5	C(22A)-
C(24A)-H(24C)	109.5	H(24A)-C(24A)-H(24C)	109.5	H(24B)-
C(24A)-H(24C)	109.5	C(27A)-C(25A)-H(25A)	107.6	C(21A)-
C(25A)-H(25A)	107.6	C(26A)-C(25A)-H(25A)	107.6	C(25A)-
C(26A)-H(26A)	109.5	C(25A)-C(26A)-H(26B)	109.5	H(26A)-
C(26A)-H(26B)	109.5	C(25A)-C(26A)-H(26C)	109.5	H(26A)-
C(26A)-H(26C)	109.5	H(26B)-C(26A)-H(26C)	109.5	C(25A)-
C(27A)-H(27A)	109.5	C(25A)-C(27A)-H(27B)	109.5	H(27A)-
C(27A)-H(27B)	109.5	C(25A)-C(27A)-H(27C)	109.5	H(27A)-
C(27A)-H(27C)	109.5	H(27B)-C(27A)-H(27C)	109.5	N(1B)-
C(1B)-H(1B)	126.0	N(2B)-C(1B)-H(1B)	126.0	C(2B)-
C(3B)-H(3B)	126.2	N(2B)-C(3B)-H(3B)	126.2	C(7B)-
C(6B)-H(6B)	119.4	C(5B)-C(6B)-H(6B)	119.4	C(6B)-

C(7B)-H(7B)	119.6	C(8B)-C(7B)-H(7B)	119.6	C(7B)-
C(8B)-H(8B)	119.5	C(9B)-C(8B)-H(8B)	119.5	C(5B)-
C(10B)-H(10B)	108.2	C(12B)-C(10B)-H(10B)	108.2	C(11B)-
C(10B)-H(10B)	108.2	C(10B)-C(11B)-H(11D)	109.5	C(10B)-
C(11B)-H(11E)	109.5	H(11D)-C(11B)-H(11E)	109.5	C(10B)-
C(11B)-H(11F)	109.5	H(11D)-C(11B)-H(11F)	109.5	H(11E)-
C(11B)-H(11F)	109.5	C(10B)-C(12B)-H(12D)	109.5	C(10B)-
C(12B)-H(12E)	109.5	H(12D)-C(12B)-H(12E)	109.5	C(10B)-
C(12B)-H(12F)	109.5	H(12D)-C(12B)-H(12F)	109.5	H(12E)-
C(12B)-H(12F)	109.5	C(9B)-C(13B)-H(13B)	107.5	C(15B)-
C(13B)-H(13B)	107.5	C(14B)-C(13B)-H(13B)	107.5	C(13B)-
C(14B)-H(14D)	109.5	C(13B)-C(14B)-H(14E)	109.5	H(14D)-
C(14B)-H(14E)	109.5	C(13B)-C(14B)-H(14F)	109.5	H(14D)-
C(14B)-H(14F)	109.5	H(14E)-C(14B)-H(14F)	109.5	C(13B)-
C(15B)-H(15D)	109.5	C(13B)-C(15B)-H(15E)	109.5	H(15D)-
C(15B)-H(15E)	109.5	C(13B)-C(15B)-H(15F)	109.5	H(15D)-
C(15B)-H(15F)	109.5	H(15E)-C(15B)-H(15F)	109.5	C(19B)-
C(18B)-H(18B)	119.5	C(17B)-C(18B)-H(18B)	119.5	C(18B)-
C(19B)-H(19B)	119.4	C(20B)-C(19B)-H(19B)	119.4	C(19B)-
C(20B)-H(20B)	119.8	C(21B)-C(20B)-H(20B)	119.8	C(17B)-
C(22B)-H(22B)	107.8	C(23B)-C(22B)-H(22B)	107.8	C(24B)-
C(22B)-H(22B)	107.8	C(22B)-C(23B)-H(23D)	109.5	C(22B)-
C(23B)-H(23E)	109.5	H(23D)-C(23B)-H(23E)	109.5	C(22B)-
C(23B)-H(23F)	109.5	H(23D)-C(23B)-H(23F)	109.5	H(23E)-
C(23B)-H(23F)	109.5	C(22B)-C(24B)-H(24D)	109.5	C(22B)-
C(24B)-H(24E)	109.5	H(24D)-C(24B)-H(24E)	109.5	C(22B)-
C(24B)-H(24F)	109.5	H(24D)-C(24B)-H(24F)	109.5	H(24E)-
C(24B)-H(24F)	109.5	C(21B)-C(25B)-H(25B)	107.6	C(27B)-
C(25B)-H(25B)	107.6	C(26B)-C(25B)-H(25B)	107.6	C(25B)-
C(26B)-H(26D)	109.5	C(25B)-C(26B)-H(26E)	109.5	H(26D)-
C(26B)-H(26E)	109.5	C(25B)-C(26B)-H(26F)	109.5	H(26D)-
C(26B)-H(26F)	109.5	H(26E)-C(26B)-H(26F)	109.5	C(25B)-
C(27B)-H(27D)	109.5	C(25B)-C(27B)-H(27E)	109.5	H(27D)-
C(27B)-H(27E)	109.5	C(25B)-C(27B)-H(27F)	109.5	H(27D)-
C(27B)-H(27F)	109.5	H(27E)-C(27B)-H(27F)	109.5	N(1C)-
C(1C)-H(1C)	125.8	N(2C)-C(1C)-H(1C)	125.8	C(2C)-
C(3C)-H(3C)	125.9	N(2C)-C(3C)-H(3C)	125.9	C(7C)-
C(6C)-H(6C)	119.1	C(5C)-C(6C)-H(6C)	119.1	C(6C)-
C(7C)-H(7C)	119.9	C(8C)-C(7C)-H(7C)	119.9	C(7C)-
C(8C)-H(8C)	119.3	C(9C)-C(8C)-H(8C)	119.3	C(5C)-
C(10C)-H(10C)	108.0	C(11C)-C(10C)-H(10C)	108.0	C(12C)-
C(10C)-H(10C)	108.0	C(10C)-C(11C)-H(11G)	109.6	C(10C)-
C(11C)-H(11H)	109.7	H(11G)-C(11C)-H(11H)	109.4	C(10C)-
C(11C)-H(11I)	109.5	H(11G)-C(11C)-H(11I)	109.2	H(11H)-
C(11C)-H(11I)	109.4	C(10C)-C(11C)-H(11X)	109.6	H(11G)-
C(11C)-H(11X)	140.8	H(11H)-C(11C)-H(11X)	56.3	H(11I)-
C(11C)-H(11X)	56.2	C(10C)-C(11C)-H(11Y)	109.5	H(11G)-
C(11C)-H(11Y)	56.1	H(11H)-C(11C)-H(11Y)	140.8	H(11I)-
C(11C)-H(11Y)	56.1	H(11X)-C(11C)-H(11Y)	109.3	C(10C)-

C(11C)-H(11Z)	109.6	H(11G)-C(11C)-H(11Z)	56.2	H(11H)-
C(11C)-H(11Z)	56.3	H(11I)-C(11C)-H(11Z)	140.8	H(11X)-
C(11C)-H(11Z)	109.5	H(11Y)-C(11C)-H(11Z)	109.3	C(10C)-
C(12C)-H(12G)	109.5	C(10C)-C(12C)-H(12H)	109.5	H(12G)-
C(12C)-H(12H)	109.5	C(10C)-C(12C)-H(12I)	109.5	H(12G)-
C(12C)-H(12I)	109.5	H(12H)-C(12C)-H(12I)	109.5	C(9C)-
C(13C)-H(13C)	107.4	C(15C)-C(13C)-H(13C)	107.4	C(14C)-
C(13C)-H(13C)	107.4	C(13C)-C(14C)-H(14G)	109.5	C(13C)-
C(14C)-H(14H)	109.5	H(14G)-C(14C)-H(14H)	109.5	C(13C)-
C(14C)-H(14I)	109.5	H(14G)-C(14C)-H(14I)	109.5	H(14H)-
C(14C)-H(14I)	109.5	C(13C)-C(15C)-H(15G)	109.5	C(13C)-
C(15C)-H(15H)	109.5	H(15G)-C(15C)-H(15H)	109.5	C(13C)-
C(15C)-H(15I)	109.5	H(15G)-C(15C)-H(15I)	109.5	H(15H)-
C(15C)-H(15I)	109.5	C(19C)-C(18C)-H(18C)	119.4	C(17C)-
C(18C)-H(18C)	119.4	C(20C)-C(19C)-H(19C)	119.7	C(18C)-
C(19C)-H(19C)	119.7	C(19C)-C(20C)-H(20C)	119.2	C(21C)-
C(20C)-H(20C)	119.2	C(23C)-C(22C)-H(22C)	109.3	C(17C)-
C(22C)-H(22C)	109.3	C(24C)-C(22C)-H(22C)	109.3	C(22C)-
C(23C)-H(23G)	109.5	C(22C)-C(23C)-H(23H)	109.5	H(23G)-
C(23C)-H(23H)	109.5	C(22C)-C(23C)-H(23I)	109.5	H(23G)-
C(23C)-H(23I)	109.5	H(23H)-C(23C)-H(23I)	109.5	C(22C)-
C(24C)-H(24G)	109.5	C(22C)-C(24C)-H(24H)	109.5	H(24G)-
C(24C)-H(24H)	109.5	C(22C)-C(24C)-H(24I)	109.5	H(24G)-
C(24C)-H(24I)	109.5	H(24H)-C(24C)-H(24I)	109.5	C(21C)-
C(25C)-H(25C)	107.5	C(27C)-C(25C)-H(25C)	107.5	C(26C)-
C(25C)-H(25C)	107.5	C(25C)-C(26C)-H(26G)	109.5	C(25C)-
C(26C)-H(26H)	109.5	H(26G)-C(26C)-H(26H)	109.5	C(25C)-
C(26C)-H(26I)	109.5	H(26G)-C(26C)-H(26I)	109.5	H(26H)-
C(26C)-H(26I)	109.5	C(25C)-C(27C)-H(27G)	109.5	C(25C)-
C(27C)-H(27H)	109.5	H(27G)-C(27C)-H(27H)	109.5	C(25C)-
C(27C)-H(27I)	109.5	H(27G)-C(27C)-H(27I)	109.5	H(27H)-
C(27C)-H(27I)	109.5	N(2D)-C(1D)-H(1D)	125.7	N(1D)-
C(1D)-H(1D)	125.7	C(2D)-C(3D)-H(3D)	126.1	N(2D)-
C(3D)-H(3D)	126.1	C(5D)-C(6D)-H(6D)	119.5	C(7D)-
C(6D)-H(6D)	119.5	C(8D)-C(7D)-H(7D)	120.0	C(6D)-
C(7D)-H(7D)	120.0	C(7D)-C(8D)-H(8D)	119.3	C(9D)-
C(8D)-H(8D)	119.3	C(5D)-C(10D)-H(10D)	107.9	C(12D)-
C(10D)-H(10D)	107.9	C(11D)-C(10D)-H(10D)	107.9	C(10D)-
C(11D)-H(11J)	109.5	C(10D)-C(11D)-H(11K)	109.5	H(11J)-
C(11D)-H(11K)	109.5	C(10D)-C(11D)-H(11L)	109.5	H(11J)-
C(11D)-H(11L)	109.5	H(11K)-C(11D)-H(11L)	109.5	C(10D)-
C(12D)-H(12J)	109.5	C(10D)-C(12D)-H(12K)	109.5	H(12J)-
C(12D)-H(12K)	109.5	C(10D)-C(12D)-H(12L)	109.5	H(12J)-
C(12D)-H(12L)	109.5	H(12K)-C(12D)-H(12L)	109.5	C(9D)-
C(13D)-H(13D)	107.9	C(15D)-C(13D)-H(13D)	107.9	C(14D)-
C(13D)-H(13D)	107.9	C(13D)-C(14D)-H(14J)	109.5	C(13D)-
C(14D)-H(14K)	109.5	H(14J)-C(14D)-H(14K)	109.5	C(13D)-
C(14D)-H(14L)	109.5	H(14J)-C(14D)-H(14L)	109.5	H(14K)-
C(14D)-H(14L)	109.5	C(13D)-C(15D)-H(15J)	109.5	C(13D)-

C(15D)-H(15K)	109.5	H(15J)-C(15D)-H(15K)	109.5	C(13D)-
C(15D)-H(15L)	109.5	H(15J)-C(15D)-H(15L)	109.5	H(15K)-
C(15D)-H(15L)	109.5	C(17D)-C(18D)-H(18D)	119.5	C(19D)-
C(18D)-H(18D)	119.5	C(20D)-C(19D)-H(19D)	119.7	C(18D)-
C(19D)-H(19D)	119.7	C(19D)-C(20D)-H(20D)	119.2	C(21D)-
C(20D)-H(20D)	119.2	C(17D)-C(22D)-H(22D)	108.0	C(24D)-
C(22D)-H(22D)	108.0	C(23D)-C(22D)-H(22D)	108.0	C(22D)-
C(23D)-H(23J)	109.5	C(22D)-C(23D)-H(23K)	109.5	H(23J)-
C(23D)-H(23K)	109.5	C(22D)-C(23D)-H(23L)	109.5	H(23J)-
C(23D)-H(23L)	109.5	H(23K)-C(23D)-H(23L)	109.5	C(22D)-
C(24D)-H(24J)	109.5	C(22D)-C(24D)-H(24K)	109.5	H(24J)-
C(24D)-H(24K)	109.5	C(22D)-C(24D)-H(24L)	109.5	H(24J)-
C(24D)-H(24L)	109.5	H(24K)-C(24D)-H(24L)	109.5	C(21D)-
C(25D)-H(25D)	108.3	C(26D)-C(25D)-H(25D)	108.3	C(27D)-
C(25D)-H(25D)	108.3	C(25D)-C(26D)-H(26J)	109.5	C(25D)-
C(26D)-H(26K)	109.5	H(26J)-C(26D)-H(26K)	109.5	C(25D)-
C(26D)-H(26L)	109.5	H(26J)-C(26D)-H(26L)	109.5	H(26K)-
C(26D)-H(26L)	109.5	C(25D)-C(27D)-H(27J)	109.5	C(25D)-
C(27D)-H(27K)	109.5	H(27J)-C(27D)-H(27K)	109.5	C(25D)-
C(27D)-H(27L)	109.5	H(27J)-C(27D)-H(27L)	109.5	H(27K)-
C(27D)-H(27L)	109.5	Cl(2S)-C(1S)-H(1SA)	109.2	Cl(1S)-
C(1S)-H(1SA)	109.2	Cl(2S)-C(1S)-H(1SB)	109.2	Cl(1S)-
C(1S)-H(1SB)	109.2	H(1SA)-C(1S)-H(1SB)	107.9	Cl(4S)-
C(2S)-H(2SA)	109.2	Cl(3S)-C(2S)-H(2SA)	109.2	Cl(4S)-
C(2S)-H(2SB)	109.2	Cl(3S)-C(2S)-H(2SB)	109.2	H(2SA)-
C(2S)-H(2SB)	107.9	Cl(6S)-C(3S)-H(3SA)	109.7	Cl(5S)-
C(3S)-H(3SA)	109.7	Cl(6S)-C(3S)-H(3SB)	109.7	Cl(5S)-
C(3S)-H(3SB)	109.7	H(3SA)-C(3S)-H(3SB)	108.2	Cl(7S)-
C(4S)-H(4SA)	109.1	Cl(8S)-C(4S)-H(4SA)	109.1	Cl(7S)-
C(4S)-H(4SB)	109.1	Cl(8S)-C(4S)-H(4SB)	109.1	H(4SA)-
C(4S)-H(4SB)	107.8			

Table 6. Torsion angles [°] for 5a.

atom-atom-atom-atom	angle	atom-atom-atom-atom	angle	
C(2A)-N(1A)-C(1A)-N(2A)	-0.3(3)	C(4A)-N(1A)-C(1A)-N(2A)	-172.1(2)	C(3A)-
N(2A)-C(1A)-N(1A)	0.6(3)	C(16A)-N(2A)-C(1A)-N(1A)	178.7(2)	C(1A)-
N(1A)-C(2A)-C(3A)	-0.2(3)	C(4A)-N(1A)-C(2A)-C(3A)	171.3(2)	C(1A)-
N(1A)-C(2A)-C(28A)	176.0(2)	C(4A)-N(1A)-C(2A)-C(28A)	-12.5(4)	N(1A)-
C(2A)-C(3A)-N(2A)	0.6(3)	C(28A)-C(2A)-C(3A)-N(2A)	-175.5(2)	C(1A)-
N(2A)-C(3A)-C(2A)	-0.8(3)	C(16A)-N(2A)-C(3A)-C(2A)	-178.8(2)	C(1A)-
N(1A)-C(4A)-C(5A)	-91.6(3)	C(2A)-N(1A)-C(4A)-C(5A)	98.1(3)	C(1A)-
N(1A)-C(4A)-C(9A)	89.0(3)	C(2A)-N(1A)-C(4A)-C(9A)	-81.3(3)	C(9A)-
C(4A)-C(5A)-C(6A)	1.0(4)	N(1A)-C(4A)-C(5A)-C(6A)	-178.3(2)	C(9A)-
C(4A)-C(5A)-C(10A)	-176.6(3)	N(1A)-C(4A)-C(5A)-C(10A)	4.1(4)	C(4A)-
C(5A)-C(6A)-C(7A)	1.6(4)	C(10A)-C(5A)-C(6A)-C(7A)	179.2(3)	C(5A)-
C(6A)-C(7A)-C(8A)	-2.6(4)	C(6A)-C(7A)-C(8A)-C(9A)	1.1(4)	C(5A)-
C(4A)-C(9A)-C(8A)	-2.4(4)	N(1A)-C(4A)-C(9A)-C(8A)	176.9(2)	C(5A)-
C(4A)-C(9A)-C(13A)	177.4(3)	N(1A)-C(4A)-C(9A)-C(13A)	-3.3(4)	C(7A)-
C(8A)-C(9A)-C(4A)	1.3(4)	C(7A)-C(8A)-C(9A)-C(13A)	-178.5(2)	C(4A)-
C(5A)-C(10A)-C(11A)	-140.8(3)	C(6A)-C(5A)-C(10A)-C(11A)	41.7(5)	C(4A)-
C(5A)-C(10A)-C(12A)	94.8(4)	C(6A)-C(5A)-C(10A)-C(12A)	-82.7(4)	C(4A)-
C(9A)-C(13A)-C(14A)	115.5(3)	C(8A)-C(9A)-C(13A)-C(14A)	-64.7(4)	C(4A)-
C(9A)-C(13A)-C(15A)	-118.9(3)	C(8A)-C(9A)-C(13A)-C(15A)	60.9(4)	C(1A)-
N(2A)-C(16A)-C(17A)	-71.5(4)	C(3A)-N(2A)-C(16A)-C(17A)	106.2(3)	C(1A)-
N(2A)-C(16A)-C(21A)	108.4(3)	C(3A)-N(2A)-C(16A)-C(21A)	-73.8(3)	C(21A)-
C(16A)-C(17A)-C(18A)	0.0(5)	N(2A)-C(16A)-C(17A)-C(18A)	179.9(3)	C(21A)-
C(16A)-C(17A)-C(22A)	179.8(3)	N(2A)-C(16A)-C(17A)-C(22A)	-0.3(5)	C(16A)-
C(17A)-C(18A)-C(19A)	-1.0(6)	C(22A)-C(17A)-C(18A)-C(19A)	179.2(4)	C(17A)-
C(18A)-C(19A)-C(20A)	1.4(7)	C(18A)-C(19A)-C(20A)-C(21A)	-0.6(6)	C(19A)-
C(20A)-C(21A)-C(16A)	-0.4(5)	C(19A)-C(20A)-C(21A)-C(25A)	-179.6(3)	C(17A)-
C(16A)-C(21A)-C(20A)	0.7(5)	N(2A)-C(16A)-C(21A)-C(20A)	-179.2(3)	C(17A)-
C(16A)-C(21A)-C(25A)	179.9(3)	N(2A)-C(16A)-C(21A)-C(25A)	0.0(4)	C(16A)-
C(17A)-C(22A)-C(24A)	118.5(4)	C(18A)-C(17A)-C(22A)-C(24A)	-61.7(6)	C(16A)-
C(17A)-C(22A)-C(23A)	-119.4(5)	C(18A)-C(17A)-C(22A)-C(23A)	60.4(6)	C(20A)-
C(21A)-C(25A)-C(27A)	96.1(3)	C(16A)-C(21A)-C(25A)-C(27A)	-83.1(3)	C(20A)-
C(21A)-C(25A)-C(26A)	-27.8(4)	C(16A)-C(21A)-C(25A)-C(26A)	153.1(3)	C(3A)-
C(2A)-C(28A)-O(1A)	173.0(3)	N(1A)-C(2A)-C(28A)-O(1A)	-2.3(4)	C(3A)-
C(2A)-C(28A)-O(2A)	-2.5(4)	N(1A)-C(2A)-C(28A)-O(2A)	-177.8(3)	C(2B)-
N(1B)-C(1B)-N(2B)	-1.3(3)	C(4B)-N(1B)-C(1B)-N(2B)	-177.9(2)	C(3B)-
N(2B)-C(1B)-N(1B)	1.5(3)	C(16B)-N(2B)-C(1B)-N(1B)	179.0(2)	C(1B)-
N(1B)-C(2B)-C(3B)	0.5(3)	C(4B)-N(1B)-C(2B)-C(3B)	177.0(2)	C(1B)-
N(1B)-C(2B)-C(28B)	179.4(2)	C(4B)-N(1B)-C(2B)-C(28B)	-4.1(4)	N(1B)-
C(2B)-C(3B)-N(2B)	0.4(3)	C(28B)-C(2B)-C(3B)-N(2B)	-178.4(3)	C(1B)-
N(2B)-C(3B)-C(2B)	-1.2(3)	C(16B)-N(2B)-C(3B)-C(2B)	-178.7(2)	C(1B)-
N(1B)-C(4B)-C(5B)	94.0(3)	C(2B)-N(1B)-C(4B)-C(5B)	-82.0(3)	C(1B)-
N(1B)-C(4B)-C(9B)	-85.3(3)	C(2B)-N(1B)-C(4B)-C(9B)	98.7(3)	C(9B)-
C(4B)-C(5B)-C(6B)	-0.2(4)	N(1B)-C(4B)-C(5B)-C(6B)	-179.5(2)	C(9B)-
C(4B)-C(5B)-C(10B)	179.9(3)	N(1B)-C(4B)-C(5B)-C(10B)	0.6(4)	C(4B)-
C(5B)-C(6B)-C(7B)	0.1(4)	C(10B)-C(5B)-C(6B)-C(7B)	180.0(3)	C(5B)-

C(6B)-C(7B)-C(8B)	-0.2(5)	C(6B)-C(7B)-C(8B)-C(9B)	0.3(5)	C(7B)-
C(8B)-C(9B)-C(4B)	-0.3(5)	C(7B)-C(8B)-C(9B)-C(13B)	-180.0(3)	C(5B)-
C(4B)-C(9B)-C(8B)	0.3(4)	N(1B)-C(4B)-C(9B)-C(8B)	179.6(3)	C(5B)-
C(4B)-C(9B)-C(13B)	179.9(3)	N(1B)-C(4B)-C(9B)-C(13B)	-0.8(4)	C(4B)-
C(5B)-C(10B)-C(12B)	-112.7(3)	C(6B)-C(5B)-C(10B)-C(12B)	67.4(4)	C(4B)-
C(5B)-C(10B)-C(11B)	123.6(4)	C(6B)-C(5B)-C(10B)-C(11B)	-56.3(4)	C(8B)-
C(9B)-C(13B)-C(15B)	-67.1(4)	C(4B)-C(9B)-C(13B)-C(15B)	113.3(4)	C(8B)-
C(9B)-C(13B)-C(14B)	58.2(6)	C(4B)-C(9B)-C(13B)-C(14B)	-121.4(5)	C(1B)-
N(2B)-C(16B)-C(21B)	-91.5(3)	C(3B)-N(2B)-C(16B)-C(21B)	85.6(3)	C(1B)-
N(2B)-C(16B)-C(17B)	91.5(3)	C(3B)-N(2B)-C(16B)-C(17B)	-91.4(3)	C(21B)-
C(16B)-C(17B)-C(18B)	-2.3(4)	N(2B)-C(16B)-C(17B)-C(18B)	174.5(2)	C(21B)-
C(16B)-C(17B)-C(22B)	175.9(2)	N(2B)-C(16B)-C(17B)-C(22B)	-7.3(4)	C(16B)-
C(17B)-C(18B)-C(19B)	0.5(4)	C(22B)-C(17B)-C(18B)-C(19B)	-177.6(3)	C(17B)-
C(18B)-C(19B)-C(20B)	0.9(4)	C(18B)-C(19B)-C(20B)-C(21B)	-0.8(5)	C(19B)-
C(20B)-C(21B)-C(16B)	-0.9(4)	C(19B)-C(20B)-C(21B)-C(25B)	175.0(3)	C(17B)-
C(16B)-C(21B)-C(20B)	2.4(4)	N(2B)-C(16B)-C(21B)-C(20B)	-174.4(2)	C(17B)-
C(16B)-C(21B)-C(25B)	-173.4(3)	N(2B)-C(16B)-C(21B)-C(25B)	9.8(4)	C(18B)-
C(17B)-C(22B)-C(23B)	-27.4(4)	C(16B)-C(17B)-C(22B)-C(23B)	154.6(2)	C(18B)-
C(17B)-C(22B)-C(24B)	95.8(3)	C(16B)-C(17B)-C(22B)-C(24B)	-82.2(3)	C(20B)-
C(21B)-C(25B)-C(27B)	-82.6(4)	C(16B)-C(21B)-C(25B)-C(27B)	93.1(3)	C(20B)-
C(21B)-C(25B)-C(26B)	42.1(4)	C(16B)-C(21B)-C(25B)-C(26B)	-142.2(3)	C(3B)-
C(2B)-C(28B)-O(1B)	160.3(3)	N(1B)-C(2B)-C(28B)-O(1B)	-18.3(4)	C(3B)-
C(2B)-C(28B)-O(2B)	-19.9(4)	N(1B)-C(2B)-C(28B)-O(2B)	161.5(3)	C(2C)-
N(1C)-C(1C)-N(2C)	-0.1(3)	C(4C)-N(1C)-C(1C)-N(2C)	-169.4(2)	C(3C)-
N(2C)-C(1C)-N(1C)	0.3(3)	C(16C)-N(2C)-C(1C)-N(1C)	-178.6(2)	C(1C)-
N(1C)-C(2C)-C(3C)	-0.2(3)	C(4C)-N(1C)-C(2C)-C(3C)	168.4(2)	C(1C)-
N(1C)-C(2C)-C(28C)	174.3(2)	C(4C)-N(1C)-C(2C)-C(28C)	-17.0(4)	N(1C)-
C(2C)-C(3C)-N(2C)	0.4(3)	C(28C)-C(2C)-C(3C)-N(2C)	-174.0(2)	C(1C)-
N(2C)-C(3C)-C(2C)	-0.5(3)	C(16C)-N(2C)-C(3C)-C(2C)	178.4(2)	C(1C)-
N(1C)-C(4C)-C(9C)	83.6(3)	C(2C)-N(1C)-C(4C)-C(9C)	-83.8(3)	C(1C)-
N(1C)-C(4C)-C(5C)	-96.0(3)	C(2C)-N(1C)-C(4C)-C(5C)	96.6(3)	C(9C)-
C(4C)-C(5C)-C(6C)	-0.2(4)	N(1C)-C(4C)-C(5C)-C(6C)	179.3(3)	C(9C)-
C(4C)-C(5C)-C(10C)	-177.3(3)	N(1C)-C(4C)-C(5C)-C(10C)	2.2(5)	C(4C)-
C(5C)-C(6C)-C(7C)	0.0(5)	C(10C)-C(5C)-C(6C)-C(7C)	177.1(3)	C(5C)-
C(6C)-C(7C)-C(8C)	0.1(5)	C(6C)-C(7C)-C(8C)-C(9C)	0.0(4)	C(5C)-
C(4C)-C(9C)-C(8C)	0.2(4)	N(1C)-C(4C)-C(9C)-C(8C)	-179.3(2)	C(5C)-
C(4C)-C(9C)-C(13C)	-178.7(3)	N(1C)-C(4C)-C(9C)-C(13C)	1.8(4)	C(7C)-
C(8C)-C(9C)-C(4C)	-0.1(4)	C(7C)-C(8C)-C(9C)-C(13C)	178.8(2)	C(6C)-
C(5C)-C(10C)-C(11C)	-83.9(4)	C(4C)-C(5C)-C(10C)-C(11C)	93.0(4)	C(6C)-
C(5C)-C(10C)-C(12C)	40.1(5)	C(4C)-C(5C)-C(10C)-C(12C)	-142.9(3)	C(4C)-
C(9C)-C(13C)-C(15C)	112.6(3)	C(8C)-C(9C)-C(13C)-C(15C)	-66.3(4)	C(4C)-
C(9C)-C(13C)-C(14C)	-121.6(3)	C(8C)-C(9C)-C(13C)-C(14C)	59.5(4)	C(1C)-
N(2C)-C(16C)-C(21C)	109.1(3)	C(3C)-N(2C)-C(16C)-C(21C)	-69.5(3)	C(1C)-
N(2C)-C(16C)-C(17C)	-72.0(3)	C(3C)-N(2C)-C(16C)-C(17C)	109.3(3)	C(21C)-
C(16C)-C(17C)-C(18C)	-1.1(5)	N(2C)-C(16C)-C(17C)-C(18C)	-179.8(3)	C(21C)-
C(16C)-C(17C)-C(22C)	179.5(3)	N(2C)-C(16C)-C(17C)-C(22C)	0.7(5)	C(16C)-
C(17C)-C(18C)-C(19C)	-0.2(6)	C(22C)-C(17C)-C(18C)-C(19C)	179.2(4)	C(17C)-
C(18C)-C(19C)-C(20C)	0.6(6)	C(18C)-C(19C)-C(20C)-C(21C)	0.4(6)	C(19C)-
C(20C)-C(21C)-C(16C)	-1.5(5)	C(19C)-C(20C)-C(21C)-C(25C)	-179.7(3)	C(17C)-

C(16C)-C(21C)-C(20C)	1.9(4)	N(2C)-C(16C)-C(21C)-C(20C)	-179.3(2)	C(17C)-	
C(16C)-C(21C)-C(25C)	-179.9(3)	N(2C)-C(16C)-C(21C)-C(25C)	-1.1(4)	C(18C)-	
C(17C)-C(22C)-C(23C)	-62.6(5)	C(16C)-C(17C)-C(22C)-C(23C)	116.8(4)	C(18C)-	
C(17C)-C(22C)-C(24C)	55.9(5)	C(16C)-C(17C)-C(22C)-C(24C)	-124.7(4)	C(20C)-	
C(21C)-C(25C)-C(27C)	-26.9(4)	C(16C)-C(21C)-C(25C)-C(27C)	155.1(3)	C(20C)-	
C(21C)-C(25C)-C(26C)	97.4(3)	C(16C)-C(21C)-C(25C)-C(26C)	-80.6(3)	C(3C)-	
C(2C)-C(28C)-O(2C)	-13.8(4)	N(1C)-C(2C)-C(28C)-O(2C)	172.9(3)	C(3C)-	
C(2C)-C(28C)-O(1C)	163.4(3)	N(1C)-C(2C)-C(28C)-O(1C)	-10.0(4)	C(3D)-	
N(2D)-C(1D)-N(1D)	-1.0(3)	C(16D)-N(2D)-C(1D)-N(1D)	178.7(2)	C(2D)-	
N(1D)-C(1D)-N(2D)	0.8(3)	C(4D)-N(1D)-C(1D)-N(2D)	177.4(2)	C(1D)-	
N(1D)-C(2D)-C(3D)	-0.3(3)	C(4D)-N(1D)-C(2D)-C(3D)	-176.7(2)	C(1D)-	
N(1D)-C(2D)-C(28D)	-179.2(2)	C(4D)-N(1D)-C(2D)-C(28D)	4.4(4)	N(1D)-	
C(2D)-C(3D)-N(2D)	-0.3(3)	C(28D)-C(2D)-C(3D)-N(2D)	178.6(3)	C(1D)-	
N(2D)-C(3D)-C(2D)	0.8(3)	C(16D)-N(2D)-C(3D)-C(2D)	-178.9(2)	C(1D)-	
N(1D)-C(4D)-C(9D)	-95.1(3)	C(2D)-N(1D)-C(4D)-C(9D)	80.8(3)	C(1D)-	
N(1D)-C(4D)-C(5D)	83.7(3)	C(2D)-N(1D)-C(4D)-C(5D)	-100.4(3)	C(9D)-	
C(4D)-C(5D)-C(6D)	0.3(4)	N(1D)-C(4D)-C(5D)-C(6D)	-178.4(3)	C(9D)-	
C(4D)-C(5D)-C(10D)	179.3(3)	N(1D)-C(4D)-C(5D)-C(10D)	0.6(4)	C(4D)-	
C(5D)-C(6D)-C(7D)	-0.6(5)	C(10D)-C(5D)-C(6D)-C(7D)	-179.6(3)	C(5D)-	
C(6D)-C(7D)-C(8D)	-0.1(5)	C(6D)-C(7D)-C(8D)-C(9D)	1.2(5)	C(5D)-	
C(4D)-C(9D)-C(8D)	0.7(4)	N(1D)-C(4D)-C(9D)-C(8D)	179.4(2)	C(5D)-	
C(4D)-C(9D)-C(13D)	179.4(3)	N(1D)-C(4D)-C(9D)-C(13D)	-1.9(4)	C(7D)-	
C(8D)-C(9D)-C(4D)	-1.5(5)	C(7D)-C(8D)-C(9D)-C(13D)	179.8(3)	C(6D)-	
C(5D)-C(10D)-C(12D)	-58.8(6)	C(4D)-C(5D)-C(10D)-C(12D)	122.2(5)	C(6D)-	
C(5D)-C(10D)-C(11D)	66.1(4)	C(4D)-C(5D)-C(10D)-C(11D)	-112.9(4)	C(4D)-	
C(9D)-C(13D)-C(15D)	-124.0(4)	C(8D)-C(9D)-C(13D)-C(15D)	54.6(5)	C(4D)-	
C(9D)-C(13D)-C(14D)	112.1(3)	C(8D)-C(9D)-C(13D)-C(14D)	-69.2(4)	C(1D)-	
N(2D)-C(16D)-C(17D)	95.8(3)	C(3D)-N(2D)-C(16D)-C(17D)	-84.5(3)	C(1D)-	
N(2D)-C(16D)-C(21D)	-85.6(3)	C(3D)-N(2D)-C(16D)-C(21D)	94.0(3)	C(21D)-	
C(16D)-C(17D)-C(18D)	-2.3(4)	N(2D)-C(16D)-C(17D)-C(18D)	176.1(2)	C(21D)-	
C(16D)-C(17D)-C(22D)	175.2(3)	N(2D)-C(16D)-C(17D)-C(22D)	-6.4(4)	C(16D)-	
C(17D)-C(18D)-C(19D)	1.5(4)	C(22D)-C(17D)-C(18D)-C(19D)	-176.1(3)	C(17D)-	
C(18D)-C(19D)-C(20D)	-0.3(5)	C(18D)-C(19D)-C(20D)-C(21D)	-0.2(5)	C(19D)-	
C(20D)-C(21D)-C(16D)	-0.6(4)	C(19D)-C(20D)-C(21D)-C(25D)	176.5(3)	C(17D)-	
C(16D)-C(21D)-C(20D)	1.9(4)	N(2D)-C(16D)-C(21D)-C(20D)	-176.5(2)	C(17D)-	
C(16D)-C(21D)-C(25D)	-175.1(3)	N(2D)-C(16D)-C(21D)-C(25D)	6.5(4)	C(16D)-	
C(17D)-C(22D)-C(24D)	145.9(3)	C(18D)-C(17D)-C(22D)-C(24D)	-36.7(4)	C(16D)-	
C(17D)-C(22D)-C(23D)	-90.5(4)	C(18D)-C(17D)-C(22D)-C(23D)	86.9(4)	C(20D)-	
C(21D)-C(25D)-C(26D)	-86.0(3)	C(16D)-C(21D)-C(25D)-C(26D)	90.8(3)	C(20D)-	
C(21D)-C(25D)-C(27D)	36.2(4)	C(16D)-C(21D)-C(25D)-C(27D)	-147.0(3)	C(3D)-	
C(2D)-C(28D)-O(1D)	-161.1(3)	N(1D)-C(2D)-C(28D)-O(1D)	17.6(4)	C(3D)-	
C(2D)-C(28D)-O(2D)	17.1(4)	N(1D)-C(2D)-C(28D)-O(2D)	-164.2(3)		

9. REFERENCES

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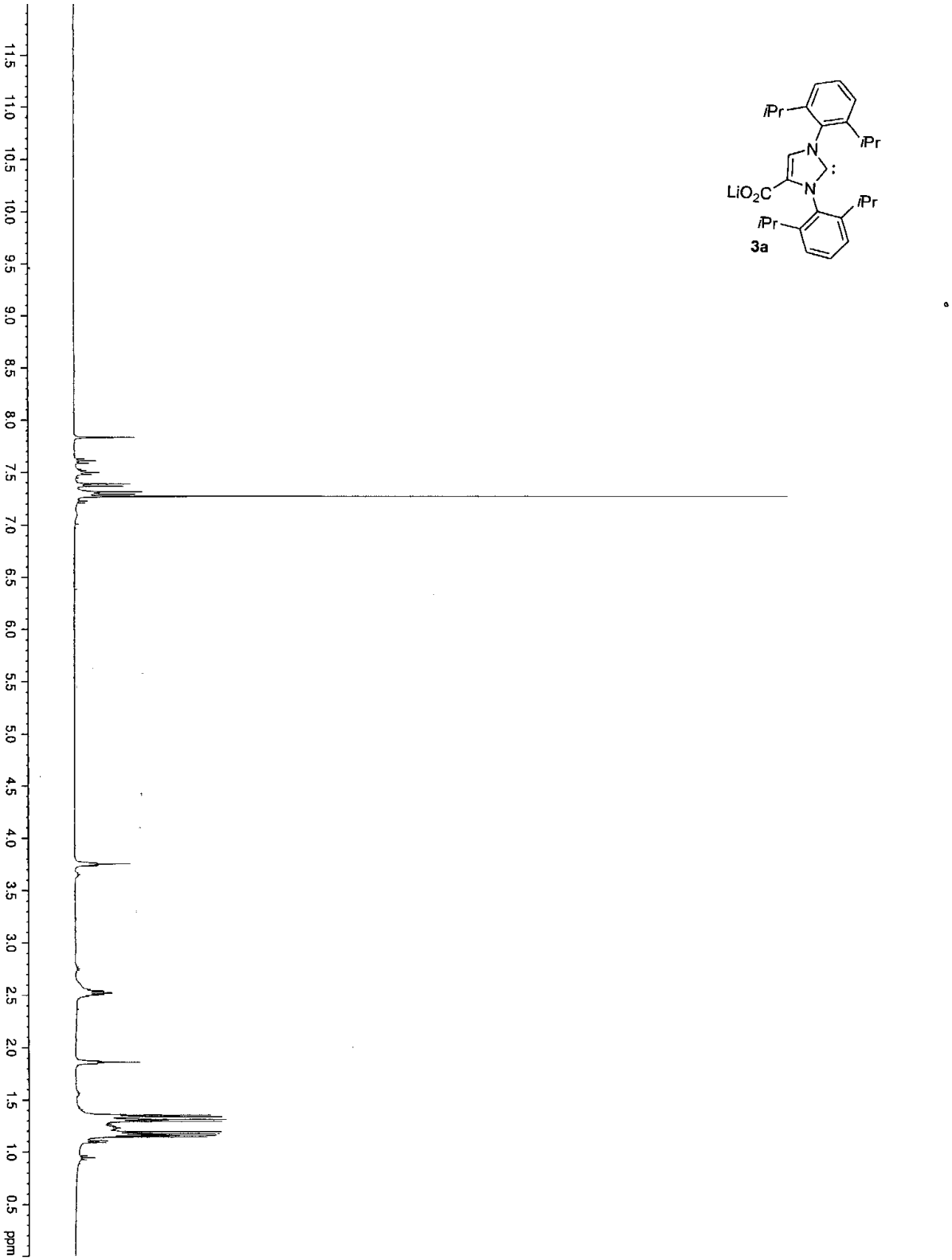
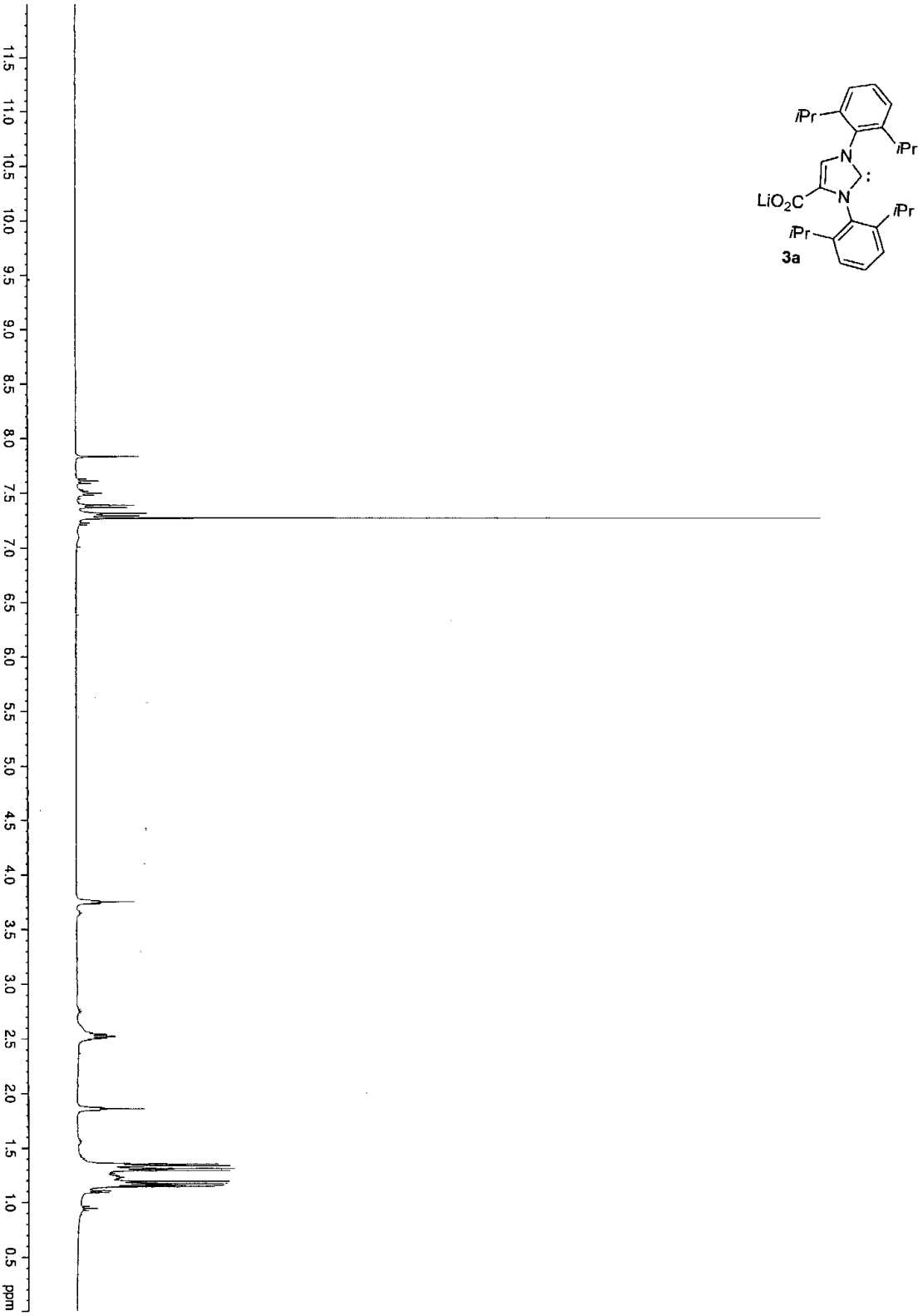
10. ^{1}H AND ^{13}C NMR SPECTRA

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ppm

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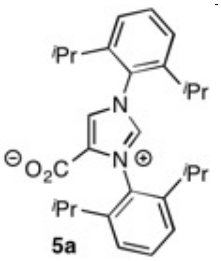
3a



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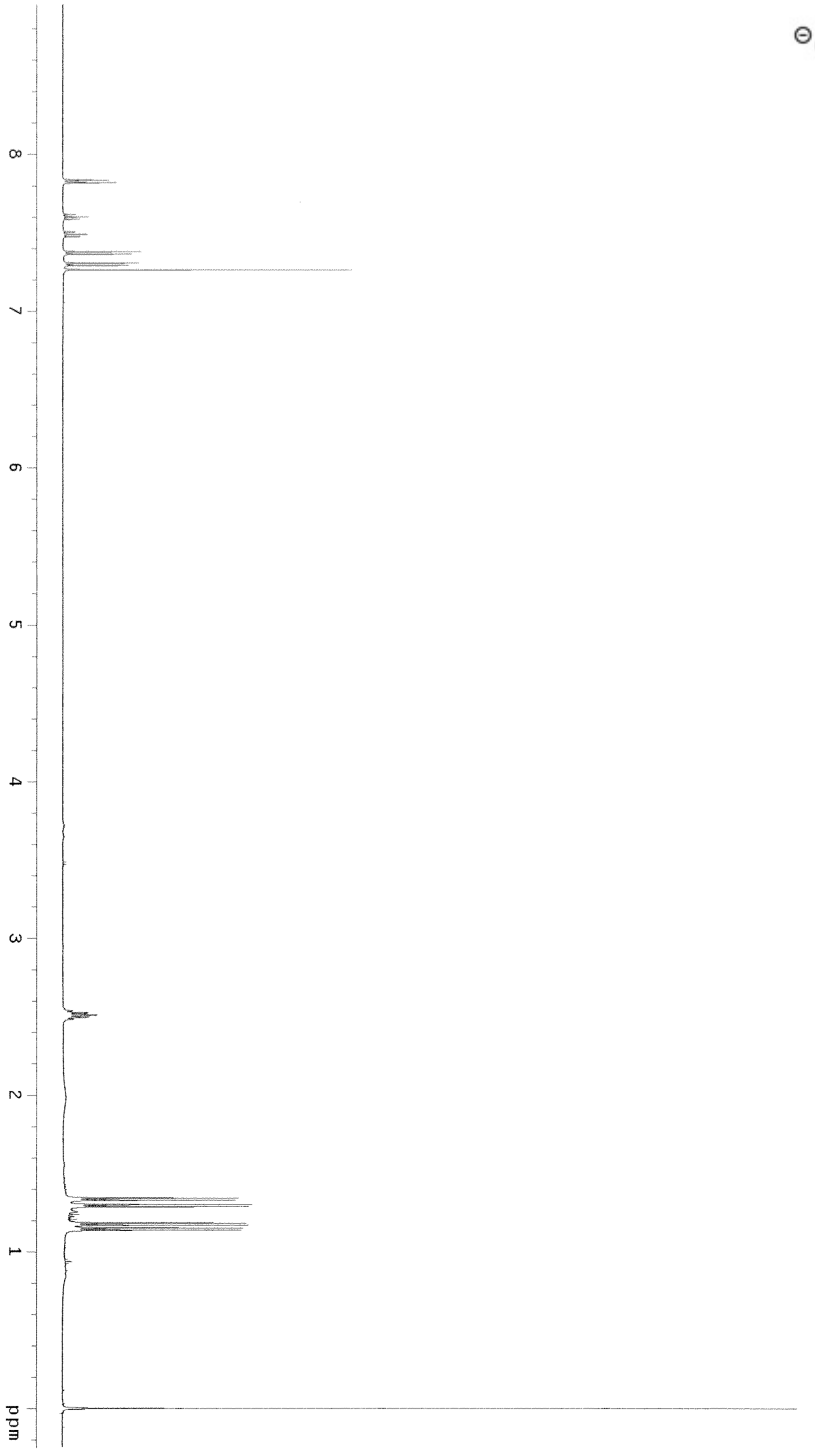

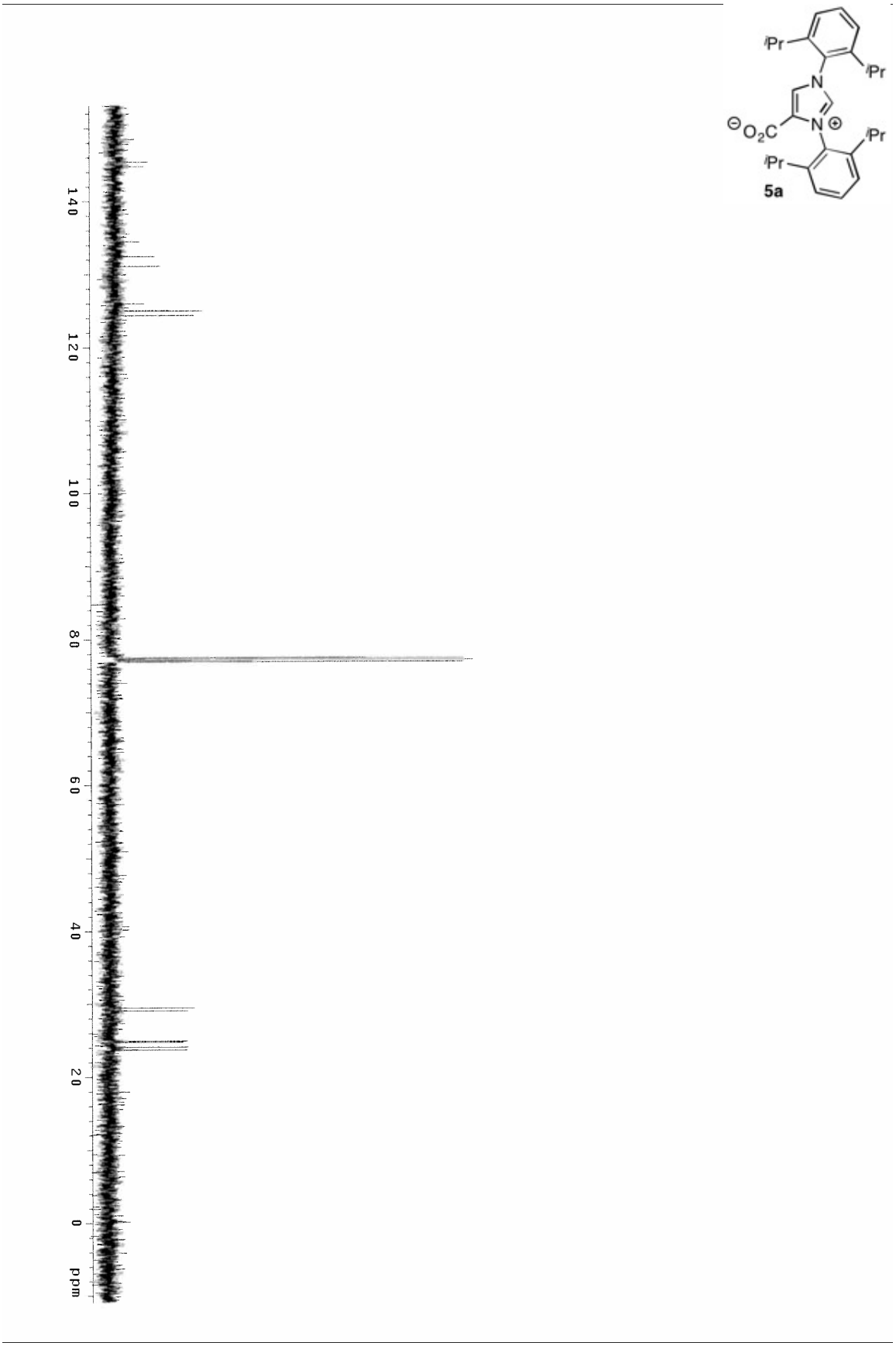

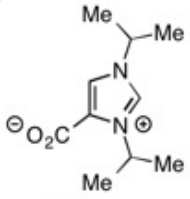

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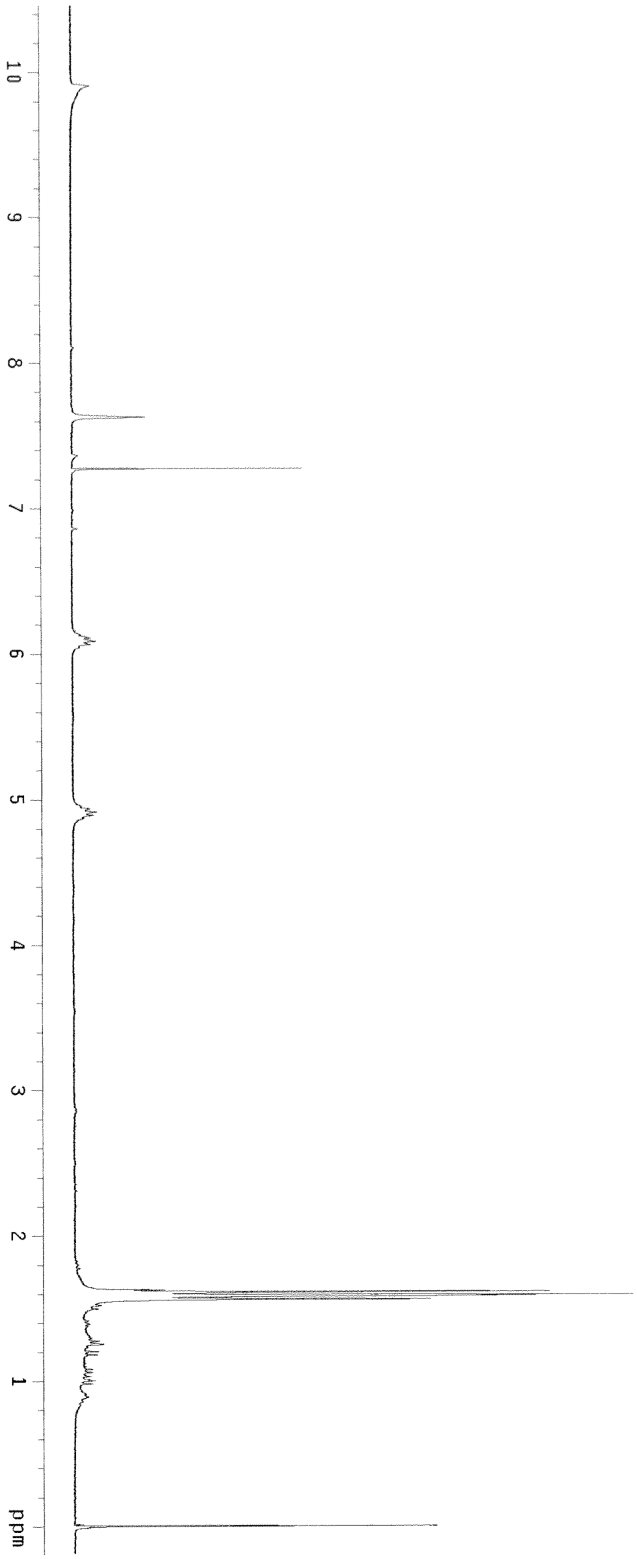

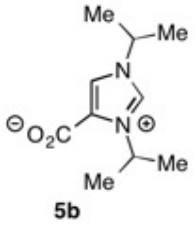

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